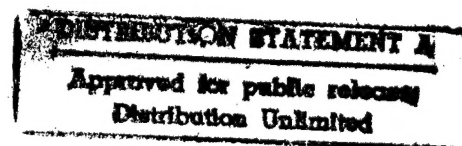19951213 006

An Improved Fast Multipole Algorithm for
Potential Fields

Tomasz Hrycak and Vladimir Rokhlin
Research Report YALEU/DCS/RR-1089
November 27, 1995

YALE UNIVERSITY
DEPARTMENT OF COMPUTER SCIENCE

A new version of the Fast Multipole Method (FMM) for potential fields is presented. While the old FMM uses multipole expansions to represent potentials, we use specially designed basis functions, displaying much faster convergence. Furthermore, we introduce an intermediate representation, in which most translation operators are diagonal. As a result, in two dimensions we obtain an improvement of a factor of three to five in speed, compared to previously published algorithms; the improvement is expected to be much greater in three dimensions. The performance of the method is illustrated with several numerical examples.

**An Improved Fast Multipole Algorithm for
Potential Fields**

Tomasz Hrycak and Vladimir Rokhlin
Research Report YALEU/DCS/RR-1089
November 27, 1995

1 Introduction

Fast Multipole Method (FMM) belongs to a class of algorithms developed for the rapid evaluation of Coulombic interactions in large-scale particle ensembles. In two dimensions, the existing implementations of the FMM rely on Taylor or Laurent (multipole) expansions for the potential field (see [2],[4]), while the three-dimensional ones are based on spherical harmonics (see [4]). The expansions, as well as the corresponding translation operators, are obtained algebraically from explicit formulas relating the Newtonian potential and its partial derivatives at various locations.

In this paper, we construct a version of the FMM based on a different analytical apparatus. Instead of multipole and Taylor expansions, we use specially designed bases, consisting of singular functions of an appropriately chosen operator. The expansions we use display much faster convergence than the previously used ones. In addition, we introduce an intermediate representation consisting of complex exponentials, and diagonalizing most translation operators. When these two techniques are combined, the resulting algorithm is about five times faster than the old one for reasonably uniform distributions, and about three times faster for highly non-uniform ones.

The structure of this paper is as follows. Section 2 introduces the mathematical preliminaries. In Section 3 we describe the analytical apparatus to be used. Section 4 contains a detailed description of the algorithm, together with its complexity analysis. Numerical experiments and the performance of the scheme are discussed in Section 5.

2 Mathematical preliminaries

2.1 Notation

For any number $s > 0$ we will denote by D_s^{in} the boundary of the square $[-\frac{s}{2}, \frac{s}{2}] \times [-\frac{s}{2}, \frac{s}{2}]$, and by D_s^{out} the boundary of the square $[-\frac{3s}{2}, \frac{3s}{2}] \times [-\frac{3s}{2}, \frac{3s}{2}]$ (see Figure 1).

We will call Ω_s^{in} the open square within the inner square D_s^{in} and Ω_s^{out} the region outside the outer square D_s^{out}. If $s = 1$, we will simply write D^{in} for D_1^{in}, D^{out} for D_1^{out}, Ω^{in} for Ω_1^{in} and Ω^{out} for Ω_1^{out}.

We will denote by B_s^{in} the set consisting of the rectangle $[-\frac{3s}{2}, \frac{7s}{2}] \times [-\frac{7s}{2}, \frac{7s}{2}]$ minus two squares $[-\frac{3s}{2}, \frac{5s}{2}] \times [-\frac{5s}{2}, \frac{7s}{2}]$ and $[-\frac{3s}{2}, \frac{5s}{2}] \times [-\frac{5s}{2}, \frac{-7s}{2}]$ (see Figure 2).

For any $s > 0$ and a complex number $z_0 = x_0 + iy_0$, we denote by Ω_{s,z_0}^{in} the open square $(x_0 - \frac{s}{2}, x_0 + \frac{s}{2}) \times (y_0 - \frac{s}{2}, y_0 + \frac{s}{2})$. Finally, we define the region Ω_{s,z_0}^{out} by the formula $\Omega_{s,z_0}^{out} = \mathbb{C} \setminus \overline{\Omega_{3s,z_0}^{in}}$.

For any set $S \subset \mathbb{R}^2$ we will denote its closure by $\overline{S}$.

In agreement with standard practice, we will denote by l^2 the Hilbert space of all complex sequences $\mathbf{x} = \{x_n\}$, such that $\sum_{n=1}^{\infty} |x_n|^2 < \infty$, with the inner product defined
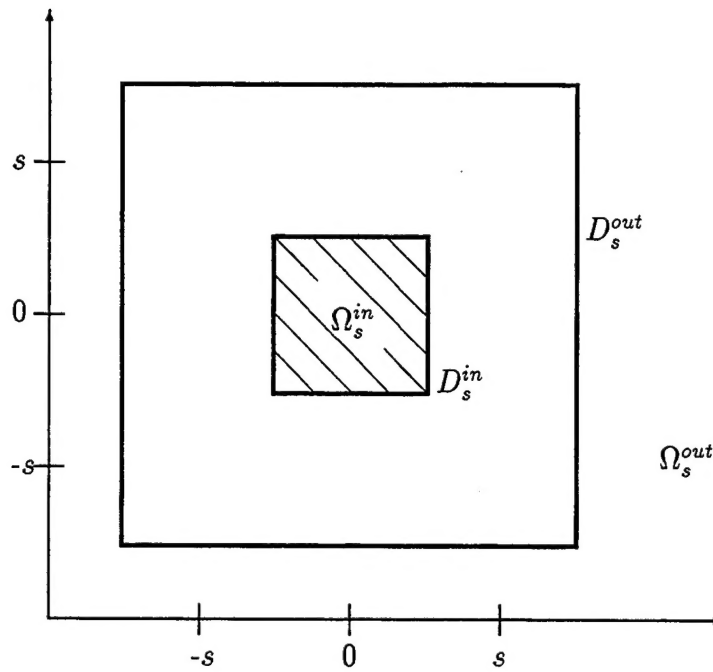
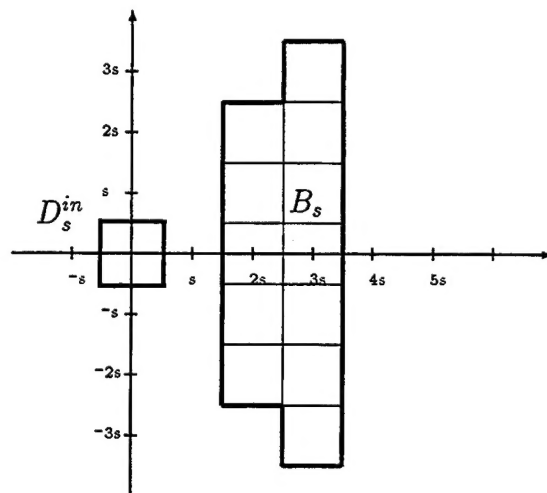Figure 1: The domains Ω_s^{in}, Ω_s^{out} and their boundaries.

Figure 2: The domain B_s.

by the formula

$$\langle \mathbf{x}, \mathbf{y} \rangle = \sum_{n=1}^{\infty} x_n \overline{y_n}. \tag{1}$$

The standard basis of l^2 will be denoted by $\mathbf{e_1}, \mathbf{e_2}, \ldots$.

Let X be a piecewise smooth curve in $\mathbb{R}^2$. A function $f : X \to \mathbb{C}$ belongs to the vector space $L^2(X)$, if and only if,

$$\|f\|_{L^2(X)} \stackrel{def}{=} \left(\int_X |f(x)|^2 \, dx \right)^{\frac{1}{2}} < \infty, \tag{2}$$

where the integration is performed with respect to the arclength dx. We say that a function $f : X \to \mathbb{C}$ belongs to the space $L^\infty(X)$, if and only if,

$$\|f\|_{L^\infty(X)} \stackrel{def}{=} \operatorname{ess\,sup}_{x \in X} |f(x)| < \infty. \tag{3}$$

2.2 Electrostatic potentials in two dimensions

In this section we list several facts from mathematical analysis, which will be used throughout the paper; all of them are either well-known, or follow immediately from well-known results.

A unit charge located at the point $\mathbf{x_0} \in \mathbb{R}^2$ generates a potential and a field given, respectively, by the expressions

$$\Phi_{\mathbf{x_0}}(\mathbf{x}) = -\log(\|\mathbf{x} - \mathbf{x_0}\|), \tag{4}$$

$$E_{\mathbf{x_0}}(\mathbf{x}) = \frac{\mathbf{x} - \mathbf{x_0}}{\|\mathbf{x} - \mathbf{x_0}\|^2}. \tag{5}$$

In this paper we will work with analytic functions of a complex variable, making no distinction between a point $\mathbf{x} = (x, y) \in \mathbb{R}^2$ and a complex number $z = x + iy$.

Since

$$\Phi_{\mathbf{x_0}}(\mathbf{x}) = -\operatorname{Re}(\log(z - z_0)), \tag{6}$$

following standard practice, we will refer to the analytic function $\log(z)$ as the potential due to a charge. To describe more complicated charge distributions we will need derivatives of $\log(z)$, and we will also refer to them as potentials.

The following lemma is an immediate consequence of the Cauchy-Riemann equations.

Lemma 2.1 *If* $f : \mathbb{C} \to \mathbb{C}$ *is analytic and*

$$u(z) = Re(f(z)), \tag{7}$$

then

$$\nabla u = (u_x, u_y) = (Re(f'), -Im(f')). \tag{8}$$

3

2.3 Hilbert-Schmidt theory for integral operators

Let X and Y be piecewise smooth curves in $\mathbb{R}^2$. We will be working with Lebesgue spaces $L^2(X)$ and $L^2(Y)$ of functions square integrable with respect to arclength measures dx and dy. The product space $L^2(X \times Y)$ consists of functions $k : X \times Y \to \mathbb{C}$, such that

$$\|k\|_{L^2(X\times Y)} = \left(\iint\limits_{X \times Y} |k(x,y)|^2 \, dx \, dy \right)^{\frac{1}{2}} < \infty. \tag{9}$$

We start with a well-known lemma (see, for example, [7], sec.VI.6).

Lemma 2.2 *If $k \in L^2(X \times Y)$, then the expression*

$$Af(x) = \int_Y k(x,y)\, f(y)\, dy \tag{10}$$

defines a continuous operator $A : L^2(Y) \to L^2(X)$, and

$$\|A\| \leq \|k\|_{L^2(X\times Y)}. \tag{11}$$

Remark 2.3 *The integral operator induced by a kernel $k \in L^2(X \times Y)$ via formula (10) is usually referred to as a Hilbert-Schmidt operator (see, for example, [7]).*

The following is an immediate consequence of Theorem VI.17. in [7]

Theorem 2.4 *If $k \in L^2(X \times Y)$, then there exist two orthonormal systems of functions $\{\phi_n\}$ in $L^2(Y)$ and $\{\psi_n\}$ in $L^2(X)$, and a sequence $\{s_n\}$, n=1,2,..., of non-negative real numbers such that*

1.
$$\sum_{n=1}^{\infty} s_n^{\,2} < \infty, \tag{12}$$

2.
$$k(x,y) = \sum_{n=1}^{\infty} s_n\, \psi_n(x)\, \overline{\phi_n(y)}, \tag{13}$$

in $L^2(X \times Y)$ sense. Moreover, the sequence $\{s_n\}$ is uniquely determined by $k \in L^2(X \times Y)$.

Theorem 2.5 (Canonical form for Hilbert-Schmidt operators)
Let $A : L^2(Y) \to L^2(X)$ be the integral operator induced by a kernel $k \in L^2(X \times Y)$ via expression (10). Then, for any $f \in L^2(Y)$,

$$Af = \sum_{n=1}^{\infty} s_n\, \langle f, \phi_n \rangle\, \psi_n, \tag{14}$$

where the functions ψ_n, ϕ_n and numbers s_n are provided by Theorem 2.4. Equivalenty,

$$A\phi_n = s_n \psi_n, \tag{15}$$

for all $n = 1,2,\ldots$.

4

Remark 2.6 A finite dimensional version of Theorem 2.4 is known in numerical analysis as the Singular Value Decomposition (SVD); the coefficients s_n are referred to as the singular values of the operator A, and the functions ψ_n and ϕ_n are called left and right singular vectors, respectively.

To restate Theorem 2.4 in these terms, we define operators $U : l^2 \to L^2(X)$ and $V : l^2 \to L^2(Y)$ by specifying them on the elements of the standard basis $\{e_n\}$ in l^2 (see Sec. 2.1), via the formulae

$$U e_n = \psi_n, \tag{16}$$

$$V e_n = \phi_n. \tag{17}$$

Now, (14) can be rewritten in the form

$$A = UDV^*, \tag{18}$$

where $D : l^2 \to l^2$ is a diagonal operator with the coefficients s_n on the diagonal, so that for all n = 1,2,...,

$$D e_n = s_n e_n. \tag{19}$$

As in the finite dimensional case, U and V are isometries.

Remark 2.7 Given an operator $A : L^2(Y) \to L^2(X)$ defined by the formula (10), the operator $A^T : L^2(X) \to L^2(Y)$ is referred to as the transpose of A if and only if for all $f \in L^2(Y)$ and $g \in L^2(X)$

$$\langle Af, \bar{g} \rangle = \langle A^T g, \bar{f} \rangle. \tag{20}$$

Similarly, the operator $A^* : L^2(X) \to L^2(Y)$ is referred to as the adjoint of A if and only if for all $f \in L^2(Y)$ and $g \in L^2(X)$

$$\langle Af, g \rangle = \langle f, A^* g \rangle. \tag{21}$$

The following well-known lemma gives explicit expressions for the operators A^T and A^* in terms of the kernel of A.

Lemma 2.8 *If an operator $A : L^2(Y) \to L^2(X)$ is defined by (10), then the operators $A^T, A^* : L^2(X) \to L^2(Y)$ are defined, respectively, by the formulae*

$$A^T f(y) = \int_X k(x,y)\, f(x)\, dx, \tag{22}$$

$$A^* f(y) = \int_X \overline{k(x,y)}\, f(x)\, dx. \tag{23}$$

The following lemma follows immediately from Lemma 2.8.

5

Lemma 2.9 *Let ψ_n and ϕ_n be the left and right singular functions the operator A defined by (10), and s_n its singular values. For each $n=1,2,\ldots$, we define the functions $\psi_n^T \in L^2(Y)$, $\phi_n^T \in L^2(X)$ via the formulae*

$$\psi_n^T = \overline{\phi_n}, \tag{24}$$

$$\phi_n^T = \overline{\psi_n}. \tag{25}$$

Then ψ_n^T and ϕ_n^T are, respectively, the left and right singular functions of A^T. Moreover,

$$A^T \phi_n^T = s_n \psi_n^T, \tag{26}$$

for all $n=1,2,\ldots$. Similarly, the functions $\psi_n^* \in L^2(Y)$, $\phi_n^* \in L^2(X)$ defined for each $n=1,2,\ldots$, via the formulae

$$\psi_n^* = \phi_n, \tag{27}$$

$$\phi_n^* = \psi_n, \tag{28}$$

are left and right singular functions of A^*, respectively. Furthermore,

$$A^* \phi_n^* = s_n \psi_n^*, \tag{29}$$

for all $n=1,2,\ldots$.

3 Analytical apparatus

3.1 Efficient representation of potentials

We will define the operators $\mathcal{C}_{out} : L^2(D^{in}) \to L^2(D^{out})$ and $\mathcal{C}_{in} : L^2(D^{out}) \to L^2(D^{in})$ by the formulae

$$\mathcal{C}_{out} f(z_2) = \int_{D^{in}} \frac{f(\xi)}{\xi - z_2} \, ds(\xi), \tag{30}$$

$$\mathcal{C}_{in} g(z_1) = \int_{D^{out}} \frac{g(\xi)}{z_1 - \xi} \, ds(\xi), \tag{31}$$

where the integration is performed with respect to the arclength ds (see Section 2.1 for the definitions of D^{in} and D^{out}). In other words, the kernel $k : D^{out} \times D^{in} \to \mathbb{C}$ of the operator $\mathcal{C}_{out}$ is given by the expression

$$k(z_2, z_1) = \frac{1}{z_1 - z_2}. \tag{32}$$

Clearly, the operators $\mathcal{C}_{out}$ and $\mathcal{C}_{in}$ satisfy the conditions of Theorem 2.4. Moreover, $\mathcal{C}_{in} = (\mathcal{C}_{out})^T$. Thus, a combination of Theorem 2.4 and Lemma 2.9 leads to the following result.

Theorem 3.1 *There exist orthonormal systems* $\{\psi_n^{out}\}$, $\{\phi_n^{in}\}$ *in* $L^2(D^{in})$ *and* $\{\psi_n^{in}\}$, $\{\phi_n^{out}\}$ *in* $L^2(D^{out})$, *and non-negative real numbers* s_n *such that*

$$\phi_n^{out} = \overline{\psi_n^{in}}, \tag{33}$$

$$\phi_n^{in} = \overline{\psi_n^{out}}, \tag{34}$$

$$\mathcal{C}_{in}\phi_n^{in} = s_n \psi_n^{in}, \tag{35}$$

$$\mathcal{C}_{out}\phi_n^{out} = s_n \psi_n^{out}, \tag{36}$$

for all $n=1,2,\ldots$ *Moreover,*

$$k(z_2, z_1) = \frac{1}{z_1 - z_2} = \sum_{n=1}^{\infty} s_n \,\psi_n^{in}(z_1)\, \psi_n^{out}(z_2). \tag{37}$$

The following theorem provides estimates for the magnitude of the singular values and singular function of the operator $\mathcal{C}_{out} : L^2(D^{in}) \to L^2(D^{out})$. Its proof is somewhat involved, and can be found in Appendix A.

Theorem 3.2 *There exist constants* $0 < q_1 < q < 1$ *and* $c > 0$, $c_1 > 0$ *such that*

$$c_1 q_1^n \leq s_n, \tag{38}$$

$$s_n \leq c q^n, \tag{39}$$

$$\|\psi_n^{in}\|_\infty \leq c n, \tag{40}$$

$$\|\psi_n^{out}\|_\infty \leq c n, \tag{41}$$

for all $n=1,2,\ldots$

Remark 3.3 Our numerical experiments show that the maximum values of the left singular functions ψ_n^{out} are uniformly bounded, while left singular functions ψ_n^{in} grow as $\log n$. Furthermore, the coefficient q in (39) is less then 0.37 (see Table 1). However, the crude estimates (38-41) are sufficient for the purposes of this paper.

The following theorem states that the left singular functions ψ_n^{out} of the operator $\mathcal{C}_{out}$ are restrictions to D^{out} of functions analytic on Ω^{out}, which are bounded at infinity. Similarly, the left singular functions ϕ_n^{in} of the operator $\mathcal{C}_{in}$ are restrictions to D^{in} of functions analytic on Ω^{in} (see Section 2.1 for definitions of D^{in}, D^{out}, Ω^{in}, and Ω^{out}).

Theorem 3.4 *Under the assumptions of Theorem 3.1, for each* $n=1,2,\ldots$, *there exist complex analytic functions* $\Psi_n^{out} : \Omega^{out} \to \mathbb{C}$ *and* $\Psi_n^{in} : \Omega^{in} \to \mathbb{C}$ *such that*

1. $\quad \Psi_n^{in}{}_{|D^{in}} = \psi_n^{in}, \tag{42}$

2. $\quad \Psi_n^{out}{}_{|D^{out}} = \psi_n^{out}, \tag{43}$

3. $\quad \lim_{|z|\to\infty} \Psi_n^{out}(z) = 0. \tag{44}$

7

Table 1: Singular values s_n of the operators C_{in} and C_{out}.

n	s_n	s_{n+1}/s_n
1	0.2359412633095143E+01	0.3475452384309655E+00
2	0.8200026261260834E+00	0.3621518314828151E+00
3	0.2969654528722792E+00	0.3761602310170769E+00
4	0.1117065933565274E+00	0.3490728065576352E+00
5	0.3899373405395550E−01	0.3641002527554371E+00
6	0.1419762842492349E−01	0.3639776390376512E+00
7	0.5167619274037499E−02	0.3642521557376765E+00
8	0.1882316460599726E−02	0.3616010580049082E+00
9	0.6806476236529151E−03	0.3635779123075419E+00
10	0.2474684420248163E−03	0.3637877346033592E+00
11	0.9002598391003066E−04	0.3642466921090881E+00
12	0.3279166684309465E−04	0.3627423712426653E+00
13	0.1189492698766364E−04	0.3637184035515401E+00
14	0.4326403854315149E−05	0.3638809145978704E+00
15	0.1574295791427948E−05	0.3641545320448064E+00
16	0.5732869472275525E−06	0.3631468873315051E+00
17	0.2081873704334665E−06	0.3638008448531035E+00
18	0.7573874125144114E−07	0.3639130712466957E+00
19	0.2756231794117075E−07	0.3640962000883560E+00
20	0.1003533522800739E−07	0.3635250072611107E+00
21	0.3646364216302235E−08	0.3638425806137019E+00
22	0.1326702566316864E−08	0.3639250220903513E+00
23	0.4828202607541905E−09	0.3640572795205558E+00
24	0.1757742306275760E−09	0.3634756451678426E+00
25	0.6388965188123934E−10	0.3638654825924015E+00
26	0.2324723901442769E−10	0.3639291306175649E+00
27	0.8460347483779406E−11	0.3640298049003309E+00
28	0.3079818643909223E−11	0.3635569373703303E+00
29	0.1119689433835681E−11	0.3638789538842048E+00
30	0.4074314198593252E−12	0.3639299339108355E+00
31	0.1482764897026021E−12	0.3640095478003274E+00
32	0.5397405796606410E−13	0.3636142130448670E+00
33	0.1962573461216843E−13	0.3638873091614348E+00
34	0.7141555758338406E−14	0.3639292924948542E+00
35	0.2599021334444648E−14	0.3639940942646556E+00
36	0.9460284166056962E−15	0.3636565040740656E+00
37	0.3440293867375512E−15	0.3638927020226409E+00
38	0.1251897831151196E−15	0.3639280307828200E+00

8

Proof. It follows from (38) that $s_n > 0$, for all n=1,2,.... Thus, (15) can be written as

$$\psi_n^{out}(z_2) = s_n^{-1} \, \mathcal{C}_{out} \phi_n^{out}(z_2) = s_n^{-1} \int_{D^{in}} \frac{\phi_n^{out}(\xi)}{\xi - z_2} \, ds(\xi), \tag{45}$$

for any $z_2 \in D^{out}$. Therefore, the formula

$$\Psi_n^{out}(z_2) = s_n^{-1} \int_{D^{in}} \frac{\phi_n^{out}(\xi)}{\xi - z_2} \, ds(\xi) \tag{46}$$

extends ψ_n^{out} to a function Ψ_n^{out} continuous on $\overline{\Omega}^{out}$ and analytic in Ω^{out}.

In a similar manner, we extend ψ_n^{in} to an analytic function on the domain Ω^{in}, continuous to the boundary D^{in}, by setting

$$\Psi_n^{in}(z_1) = s_n^{-1} \, \mathcal{C}_{in} \phi_n^{in}(z_1) = s_n^{-1} \int_{D^{out}} \frac{\phi_n^{in}(\xi)}{z_1 - \xi} \, ds(\xi). \tag{47}$$

$\square$

Given a charge anywhere in the region Ω^{in}, the following two theorems allow us to represent its potential inside the region Ω^{out} by a linear combination of left singular functions ψ_n^{out} of the operator $\mathcal{C}_{out}$. Similarly, the potential of a charge in the region Ω^{out} can be expressed inside the region Ω^{in} as a linear combination of left singular functions ψ_n^{in} of the operator $\mathcal{C}_{in}$.

Theorem 3.5 *For any $z_1 \in D^{in}$, $z_2 \in D^{out}$,*

$$\frac{1}{z_1 - z_2} = \sum_{n=1}^{\infty} s_n \psi_n^{in}(z_1) \, \psi_n^{out}(z_2). \tag{48}$$

Moreover, there exists a constant $c_1 > 0$, such that for any $z_1 \in D^{in}$, $z_2 \in D^{out}$ and integer $N > 0$

$$\left| \frac{1}{z_1 - z_2} - \sum_{n=1}^{N} s_n \psi_n^{in}(z_1) \, \psi_n^{out}(z_2) \right| \le c_1 \, N^2 \, q^N. \tag{49}$$

Proof. Let us define S_N, N=1,2,..., by the formula

$$S_N = \sum_{n=1}^{N} s_n \, \psi_n^{in} \, \psi_n^{out}. \tag{50}$$

It follows immediately from Theorem 3.2, that for there exists a constant $c_1 > 0$, such that for any integers $M > N > 0$,

$$\|S_M - S_N\|_\infty = \| \sum_{n=N+1}^{M} s_n \, \psi_n^{in} \, \psi_n^{out} \|_\infty \le \sum_{n=N+1}^{M} s_n \|\psi_n^{in}\|_\infty \|\psi_n^{out}\|_\infty$$

$$\le \sum_{n=N+1}^{\infty} c^3 \, n^2 \, q^n \le c_1 \, N^2 \, q^N. \tag{51}$$

9

Since $c_1 N^2 q^N \to 0$ as $N \to \infty$, the sequence $\{S_N\}$ of continuous functions $\sum_{n=1}^{\infty} s_n \psi_n^{in} \psi_n^{out}$ converges in the maximum norm to a limit, which we denote by S. Due to Theorem 2.4, $\{S_N\}$ converges to the function $\frac{1}{z_1 - z_2}$ in $L^2(D^{out} \times D^{in})$, so we have

$$S(z_2, z_1) = \frac{1}{z_1 - z_2}, \tag{52}$$

for all $z_1 \in D^{in}$, $z_2 \in D^{out}$. Thus, from (51) and (52) we obtain

$$\| \frac{1}{z_1 - z_2} - \sum_{n=1}^{N} s_n \psi_n^{in} \psi_n^{out} \|_\infty = \| S - S_N \|_\infty = \| \lim_{M \to \infty} S_M - S_N \|_\infty \le c_1 N^2 q^N. \tag{53}$$

$\square$

Theorem 3.6 *For any $z_1 \in \Omega^{in}$, $z_2 \in \Omega^{out}$,*

$$\frac{1}{z_1 - z_2} = \sum_{n=1}^{\infty} s_n \Psi_n^{in}(z_1) \Psi_n^{out}(z_2). \tag{54}$$

Furthermore, there exists a constant $c_1 > 0$, such that for any $z_1 \in \Omega^{in}$, $z_2 \in \Omega^{out}$, and integer $N > 0$,

$$| \frac{1}{z_1 - z_2} - \sum_{n=1}^{N} s_n \Psi_n^{in}(z_1) \Psi_n^{out}(z_2) | \le c_1 N^2 q^N. \tag{55}$$

Proof. Due to a combination of the maximum modulus principle for complex analytic functions and (49), we have

$$\max_{z_1 \in \Omega^{in}} \max_{z_2 \in \Omega^{out}} | \frac{1}{z_1 - z_2} - \sum_{n=1}^{N} s_n \Psi_n^{in}(z_1) \Psi_n^{out}(z_2) | =$$

$$\max_{z_1 \in D^{in}} \max_{z_2 \in D^{out}} | \frac{1}{z_1 - z_2} - \sum_{n=1}^{N} s_n \Psi_n^{in}(z_1) \Psi_n^{out}(z_2) | =$$

$$\max_{z_1 \in D^{in}} \max_{z_2 \in D^{out}} | \frac{1}{z_1 - z_2} - \sum_{n=1}^{N} s_n \psi_n^{in}(z_1) \psi_n^{out}(z_2) | \le c_1 N^2 q^N, \tag{56}$$

which proves (55), and (54) follows from (55) immediately. $\square$

Let Ψ_n^{in} and Ψ_n^{out} be the functions provided by Theorem 3.4. For any real number $s > 0$ and point $z_0 \in \Omega_s^{in}$, we define analytic functions $\Psi_{n,s,z_0}^{in} : \Omega_{s,z_0}^{in} \to \mathbb{C}$ and $\Psi_{n,s,z_0}^{out} : \Omega_{s,z_0}^{out} \to \mathbb{C}$, n=1,2,..., by the formulae

$$\Psi_{n,s,z_0}^{in}(z_1) = \frac{1}{\sqrt{s}} \Psi_n^{in}(\frac{z_1 - z_0}{s}), \tag{57}$$

10

$$\Psi_{n,s,z_0}^{out}(z_2) = \frac{1}{\sqrt{s}} \, \Psi_n^{out}(\frac{z_2 - z_0}{s}), \tag{58}$$

for all $z_1 \in \Omega_{s,z_0}^{in}$ and all $z_2 \in \Omega_{s,z_0}^{out}$. Moreover, suppose that ψ_n^{in} and ψ_n^{out} are the functions provided by Theorem 3.1. For any real number $s > 0$ and point $z_0 \in D_s^{in}$, we define functions $\psi_{n,s,z_0}^{in} : D_{s,z_0}^{in} \to \mathbb{C}$ and $\psi_{n,s,z_0}^{out} : D_{s,z_0}^{out} \to \mathbb{C}$, n=1,2,..., by the formulae

$$\psi_{n,s,z_0}^{in}(z_1) = \frac{1}{\sqrt{s}} \, \psi_n^{in}(\frac{z_1 - z_0}{s}), \tag{59}$$

$$\psi_{n,s,z_0}^{out}(z_2) = \frac{1}{\sqrt{s}} \, \psi_n^{out}(\frac{z_2 - z_0}{s}), \tag{60}$$

for all $z_1 \in D_{s,z_0}^{in}$ and all $z_2 \in D_{s,z_0}^{out}$ (see Section 2.1 for definitions of $D_{s,z_0}^{in}, D_{s,z_0}^{out}$, $\Omega_{s,z_0}^{in}, \Omega_{s,z_0}^{out}$).

The following theorem is an immediate consequence of Theorem 3.6 and Theorem 3.1.

Theorem 3.7 *Suppose that $s > 0$ is a real number and $z_0 \in D_s^{in}$. Then*
1. The functions $\{\psi_{n,s,z_0}^{in}\}$ form an orthonormal system in $L^2(D_{s,z_0}^{in})$. The functions $\{\psi_{n,s,z_0}^{out}\}$ form an orthonormal system in $L^2(D_{s,z_0}^{out})$.
2. $\quad \Psi_{n,s,z_0}^{out} \big|_{D_{s,z_0}^{out}} = \psi_{n,s,z_0}^{out}, \; n = 1,2,\ldots$
3. For any $z_1 \in \Omega_{s,z_0}^{in}$, $z_2 \in \Omega_{s,z_0}^{out}$,

$$\frac{1}{z_1 - z_2} = \sum_{n=1}^{\infty} s_n \Psi_{n,s,z_0}^{in}(z_1) \, \Psi_{n,s,z_0}^{out}(z_2). \tag{61}$$

Furthermore, there exist constants $c > 0$, $0 < q < 1$ such that for any $s > 0$, $z_1 \in \Omega_{s,z_0}^{in}$, $z_2 \in \Omega_{s,z_0}^{out}$, and integer $N > 0$,

$$\left| \frac{1}{z_1 - z_2} - \sum_{n=1}^{N} s_n \Psi_{n,s,z_0}^{in}(z_1) \, \Psi_{n,s,z_0}^{out}(z_2) \right| \leq \frac{c}{s} \, N^2 \, q^N. \tag{62}$$

The following two theorems are immediate consequences of Theorem 3.7.

Theorem 3.8 *Suppose that*

$$\Phi(z) = \sum_{i=1}^{m} \frac{q_i}{z_i - z} \tag{63}$$

is the potential due to a set of m charges of strengths $q_1, q_2, \ldots, q_m$ located at points $z_1, z_2, \ldots, z_m$ inside the square Ω_{s,z_0}^{in}. Suppose further that the functions $\Psi_{n,s,z_0}^{in} : \Omega_{s,z_0}^{in} \to \mathbb{C}$, $\Psi_{n,s,z_0}^{out} : \Omega_{s,z_0}^{out} \to \mathbb{C}$ are defined by the formulae (57), (58), and s_n are defined by (37). Then for any $z \in \Omega_{s,z_0}^{out}$,

$$\Phi(z) = \sum_{n=1}^{\infty} a_n \Psi_{n,s,z_0}^{out}(z), \tag{64}$$

11

with

$$a_n = s_n \sum_{i=1}^{m} q_i \, \Psi_{n,s,z_0}^{in}(z_i), \tag{65}$$

for all $n = 1, 2, \ldots$. *Furthermore, there exist constants* $c > 0$ *and* $0 < q < 1$, *such that for any real number* $s > 0$, *integer* $N > 0$ *and* $z \in \Omega_{s,z_0}^{out}$,

$$\left| \Phi(z) - \sum_{n=1}^{N} a_n \Psi_{n,s,z_0}^{out}(z) \right| \le \frac{c}{s} N^2 q^N \sum_{i=1}^{m} |q_i|. \tag{66}$$

Theorem 3.9 *Suppose that* Φ *given by the formula (63) is the potential due to a set of* m *charges of strengths* $q_1, q_2, \ldots, q_m$ *located at points* $z_1, z_2, \ldots, z_m$ *inside the region* Ω_{s,z_0}^{out}. *Suppose further that the functions* $\Psi_{n,s,z_0}^{in} : \Omega_{s,z_0}^{in} \to \mathbb{C}$, $\Psi_{n,s,z_0}^{out} : \Omega_{s,z_0}^{out} \to \mathbb{C}$ *are defined by the formulae (57), (58), and* s_n *are defined by (37). Then for any* $z \in \Omega_{s,z_0}^{in}$,

$$\Phi(z) = \sum_{n=1}^{\infty} a_n \Psi_{n,s,z_0}^{in}(z), \tag{67}$$

with

$$a_n = -s_n \sum_{i=1}^{m} q_i \, \Psi_{n,s,z_0}^{out}(z_i), \tag{68}$$

for all $n = 1, 2, \ldots$. *Furthermore, there exist constants* $c > 0$ *and* $0 < q < 1$, *such that for any real number* $s > 0$ *integer* $N > 0$ *and* $z \in \Omega_{s,z_0}^{in}$,

$$\left| \Phi(z) - \sum_{n=1}^{N} a_n \Psi_{n,s,z_0}^{in}(z) \right| \le \frac{c}{s} N^2 q^N \sum_{i=1}^{m} |q_i|. \tag{69}$$

3.2 Translation Operators and Error Bounds

The following five theorems allow us to translate expansions of the forms (64), (67) from one center z_0 to another, and to convert expansions of the form (64) into expansions of the form (67). We only provide proofs of Theorems 3.10, 3.11, 3.16 below; the proofs of Theorems 3.12, 3.14 are virtually identical to the proof of Theorem 3.10, while the proofs of Theorems 3.13, 3.15 are identical to the proof of Theorem 3.11. Thus, the proofs of Theorems 3.12, 3.13, 3.14, 3.15 are omitted.

For a real number $s > 0$ and a point $z_0 \in \Omega_s^{in}$, we define coefficients p_{n,k,s,z_0}^{out} and p_{n,k,s,z_0}^{in}, respectively, by the formulae

$$p_{n,k,s,z_0}^{out} = \int_{D_{2s,0}^{out}} \Psi_{k,s,z_0}^{out}(\xi) \, \overline{\Psi_{n,2s,0}^{out}(\xi)} \, ds(\xi), \tag{70}$$

$$p_{n,k,s,z_0}^{in} = \int_{D_{2s,0}^{in}} \Psi_{k,s,z_0}^{in}(\xi) \, \overline{\Psi_{n,2s,0}^{in}(\xi)} \, ds(\xi), \tag{71}$$

with $k = 1, 2, \ldots$, and $n = 1, 2, \ldots$.

Theorem 3.10 *Suppose that Φ defined by the formula (63) is the potential due to a set of m charges of strengths $q_1, q_2, \ldots, q_m$ located in the square Ω^{in}_{s,z_0}, and Ψ^{out}_{n,s,z_0} are functions defined by (58), with $n = 1,2,\ldots$. Suppose further that*

$$\Phi(z) = \sum_{n=1}^{\infty} a_n \Psi^{out}_{n,s,z_0}(z), \tag{72}$$

$$\Phi(z) = \sum_{n=1}^{\infty} b_n \Psi^{out}_{n,2s,0}(z), \tag{73}$$

are the expansions provided by Theorem 3.8 valid in Ω^{out}_{s,z_0} and $\Omega^{out}_{2s,0}$, respectively. Then for $n = 1,2,\ldots$

$$b_n = \sum_{k=1}^{\infty} p^{out}_{n,k,s,z_0} a_k, \tag{74}$$

with the coefficients p^{out}_{n,k,s,z_0} defined by (70).

Proof. Since the functions $\{\psi^{out}_{n,2s,0}\}$ form an orthonormal system in $L^2(D^{out}_{2s,0})$,

$$b_n = \int_{D^{out}_{2s,0}} \sum_{k=1}^{\infty} b_k \psi^{out}_{k,2s,0}(z) \overline{\psi^{out}_{n,2s,0}(z)} ds(z) \tag{75}$$

$$= \int_{D^{out}_{2s,0}} \sum_{k=1}^{\infty} a_k \Psi^{out}_{k,s,z_0}(z) \overline{\Psi^{out}_{n,2s,0}(z)} ds(z) = \sum_{k=1}^{\infty} p^{out}_{n,k,s,,z_0} a_k, \tag{76}$$

for n = 1,2,.... $\qquad\qquad\square$

Theorem 3.11 *Suppose that under the conditions of Theorem 3.10, $N > 0$ is an integer and coefficients b_n^N $(n = 1,2,\ldots,N)$, are defined by the formula*

$$b_n^N = \sum_{k=1}^{N} p^{out}_{n,k,s,z_0} a_k, \tag{77}$$

with p^{out}_{n,k,s,z_0} defined by (70). Then there exist constants $c > 0$ and $0 < q < 1$, such that for any $s > 0$, $N > 0$ and $z \in \Omega^{out}_{2s}$,

$$|\Phi(z) - \sum_{n=1}^{N} b_n^N \Psi^{out}_{n,s,0}(z)| \leq \frac{c}{s} N^4 q^N \sum_{i=1}^{m} |q_i|. \tag{78}$$

Proof. Let $0 < q < 1$ be the constant provided by Theorem 3.8. Clearly, it is sufficient to show that

$$|\sum_{n=1}^{N} b_n \Psi^{out}_{n,s,0}(z) - \sum_{n=1}^{N} b_n^N \Psi^{out}_{n,s,0}(z)| \leq \frac{c}{s} N^4 q^N \sum_{i=1}^{m} |q_i|, \tag{79}$$

13

for some constant $c > 0$. Now, by a combination of (39), (40), (41) and (65),

$$| \sum_{n=1}^{N} b_n \Psi_{n,s,0}^{out}(z) - \sum_{n=1}^{N} b_n^N \Psi_{n,s,0}^{out}(z)| = | \sum_{n=1}^{N} (b_n - b_n^N) \Psi_{n,s,0}^{out}(z)|$$

$$= | \sum_{n=1}^{N} \Psi_{n,s,0}^{out}(z) \sum_{k=N+1}^{\infty} p_{n,k,s,z_0}^{out} a_k| \leq \sum_{n=1}^{N} c_1 \frac{n}{\sqrt{s}} \sum_{k=N+1}^{\infty} |p_{n,k,s,z_0}^{out}| s_k \frac{n}{\sqrt{s}} \sum_{i=1}^{m} |q_i|$$

$$\leq \frac{c_2}{s} N^2 \sum_{i=1}^{m} |q_i| \sum_{n=1}^{N} \sum_{k=N+1}^{\infty} |p_{n,k,s,z_0}^{out}| \, q^k, \tag{80}$$

for some constants $c_1 > 0$, $c_2 > 0$. Due to Schwarz's inequality and (41), there exists $c_3 > 0$, such that for all positive integers k and n

$$|p_{n,k,s,z_0}^{out}| \leq \|\Psi_{k,s,z_0}^{out}\|_{L^2(D_{2s,0}^{out})} \|\Psi_{n,2s,0}^{out}\|_{L^2(D_{2s,0}^{out})} \leq c_3 \, k. \tag{81}$$

Now (79) follows from (80) and (81). $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\quad\square$

Theorem 3.12 *Suppose that Φ defined by the formula (63) is the potential due to a set of m charges of strengths $q_1, q_2, \ldots, q_m$ located in the square Ω_{s,z_0}^{out}, and Ψ_{n,s,z_0}^{in} are functions defined by (57), with $n = 1, 2, \ldots$. Suppose further that*

$$\Phi(z) = \sum_{n=1}^{\infty} a_n \Psi_{n,2s,0}^{in}(z) \tag{82}$$

$$\Phi(z) = \sum_{n=1}^{\infty} b_n \Psi_{n,s,z_0}^{in}(z), \tag{83}$$

are the expansions provided by Theorem 3.9 valid in $\Omega_{2s,0}^{in}$ and Ω_{s,z_0}^{in}, respectively. Then for $n = 1, 2, \ldots$ formula

$$b_n = \sum_{k=1}^{\infty} p_{n,k,s,z_0}^{in} a_k, \tag{84}$$

with the coefficients p_{n,k,s,z_0}^{in} defined by (71).

Theorem 3.13 *Suppose that under the conditions of Theorem 3.12, $N > 0$ is an integer and coefficients b_n^N ($n = 1, 2, \ldots, N$), are defined by the formula*

$$b_n^N = \sum_{k=1}^{N} p_{n,k,s,z_0}^{in} a_k, \tag{85}$$

with p_{n,k,s,z_0}^{in} defined by (71). Then there exist constants $c > 0$ and $0 < q < 1$, such that for any $s > 0$, integer $N > 0$ and $z \in \Omega_{2s}^{in}$,

$$|\Phi(z) - \sum_{n=1}^{N} b_n^N \Psi_{n,s,0}^{in}(z)| \leq \frac{c}{s} N^4 q^N \sum_{i=1}^{m} |q_i|. \tag{86}$$

Suppose that $s > 0$ is a real number and $z_0 \in \Omega_{4s}^{out}$. For k = 1,2,..., and n = 1,2,...,
we define coefficients q_{n,k,s,z_0} by the formula

$$q_{n,k,s,z_0} = \int_{D_s^{in}} \Psi_{k,s,0}^{out}(\xi) \, \overline{\Psi_{n,s,z_0}^{in}(\xi)} \, ds(\xi). \tag{87}$$

Theorem 3.14 *Suppose that Φ defined by the formula (63) is the potential due to a set
of m charges of strengths $q_1, q_2, \ldots, q_m$ located in the square Ω_s^{in}, and Ψ_{n,s,z_0}^{out}, Ψ_{n,s,z_0}^{in} are
functions defined by (58) and (57), respectively. Suppose further that*

$$\Phi(z) = \sum_{n=1}^{\infty} a_n \Psi_{n,s,0}^{out}(z), \tag{88}$$

$$\Phi(z) = \sum_{n=1}^{\infty} b_n \Psi_{n,s,z_0}^{in}(z), \tag{89}$$

*are the expansions provided by Theorem 3.8 and Theorem 3.9 valid in $\Omega_{s,0}^{out}$ and Ω_{s,z_0}^{in},
respectively. Then for all n = 1,2,... the formula*

$$b_n = \sum_{k=1}^{\infty} q_{n,k,s,z_0} \, a_k, \tag{90}$$

with the coefficients q_{n,k,s,z_0} defined by (87).

Theorem 3.15 *Suppose that under the conditions of Theorem 3.10, $N > 0$ is an integer
and coefficients b_n^N (n = 1,2,...,N), are defined by the formula*

$$b_n^N = \sum_{k=1}^{N} q_{n,k,s,z_0} \, a_k, \tag{91}$$

*with q_{n,k,s,z_0} defined by (87). Then there exist constants $c > 0$ and $0 < q < 1$, such that
for any $s > 0$, integer $N > 0$ and $z \in \Omega_{2s}^{out}$,*

$$|\Phi(z) - \sum_{n=1}^{N} b_n^N \Psi_{n,s,0}^{out}(z)| \le \frac{c}{s} N^4 q^N \sum_{i=1}^{m} |q_i|. \tag{92}$$

The following two theorems list certain properties of the coefficients p_{n,k,s,z_0}^{in}, p_{n,k,s,z_0}^{out}
and q_{n,k,s,z_0}. They are quite similar, and we only prove the first one.

Theorem 3.16 *Suppose that $s > 0$ is a real number, $z_0 \in \Omega_s^{in}$, and the coefficients
p_{n,k,s,z_0}^{out}, p_{n,k,s,z_0}^{in} are defined by formulae (70) and (71). Then*

$$p_{n,k,s,z_0}^{out} = p_{n,k,1,\frac{z_0}{s}}^{out}, \tag{93}$$

$$p_{n,k,s,z_0}^{in} = p_{n,k,1,\frac{z_0}{s}}^{in}, \tag{94}$$

$$p_{n,k,s,z_0}^{out} = p_{k,n,s,z_0}^{in}, \tag{95}$$

with any k = 1,2,..., n = 1,2,....

Proof. Due to (58) and (70)

$$
\begin{aligned}
p_{n,k,s,z_0}^{out} &= \int_{D_{2s,0}^{out}} \Psi_{k,s,z_0}^{out}(\xi)\, \overline{\Psi_{n,2s,0}^{out}(\xi)}\, ds(\xi) \\
&= \int_{D_{2s,0}^{out}} \frac{1}{\sqrt{s}}\, \Psi_k^{out}\Big(\frac{\xi - z_0}{s}\Big) \frac{1}{\sqrt{2s}}\, \overline{\Psi_n^{out}\Big(\frac{\xi}{2s}\Big)}\, ds(\xi) \\
&= \int_{D_{2,0}^{out}} \Psi_k^{out}\Big(\xi - \frac{z_0}{s}\Big) \frac{1}{\sqrt{2}}\, \overline{\Psi_n^{out}\Big(\frac{\xi}{2}\Big)}\, ds(\xi) \\
&= p_{k,n,1,\frac{z_0}{s}}^{out},
\end{aligned}
\tag{96}
$$

which proves (93). The proof of (94) is identical.

Turning our attention to (95), we observe that due to Theorem 3.1,

$$
\begin{aligned}
p_{n,k,1,\frac{z_0}{s}}^{out} &= \int_{D_{2,0}^{out}} \Psi_k^{out}\Big(\xi - \frac{z_0}{s}\Big) \frac{1}{\sqrt{2}}\, \overline{\Psi_n^{out}\Big(\frac{\xi}{2}\Big)}\, ds(\xi) \\
&= \int_{D_{2,0}^{out}} \overline{\Phi_k^{in}\Big(\xi - \frac{z_0}{s}\Big) \frac{1}{\sqrt{2}} \frac{1}{s_n} \mathcal{C}_{out}\Phi_n^{out}\Big(\frac{\xi}{2}\Big)}\, ds(\xi) \\
&= \int_{D_{2,0}^{in}} \overline{\frac{1}{\sqrt{2}} \frac{1}{s_n} \mathcal{C}_{in}\Phi_k^{in}\Big(\frac{\xi}{2}\Big)}\, \Phi_n^{out}\Big(\xi - \frac{z_0}{s}\Big)\, ds(\xi) \\
&= \int_{D_{2,0}^{in}} \overline{\frac{1}{\sqrt{2}}\Psi_k^{in}\Big(\frac{\xi}{2}\Big)}\, \Psi_n^{in}\Big(\xi - \frac{z_0}{s}\Big)\, ds(\xi) \\
&= p_{k,n,1,\frac{z_0}{s}}^{in},
\end{aligned}
\tag{97}
$$

and (95) follows directly from (93), (94) and (97). $\qquad\square$

Theorem 3.17 *Suppose that $s > 0$ is a real number, z_0 is an arbitrary point in Ω_{4s}^{out}, and the coefficients q_{n,k,s,z_0} are defined by formula (87). Then*

$$
q_{n,k,s,z_0} = q_{n,k,1,\frac{z_0}{s}},
\tag{98}
$$

for all $k = 1,2,\ldots$, $n = 1,2,\ldots$.

3.3 Diagonal Form of Translation Operators

In this section we construct a representation of potentials (63) in which the translation operators are diagonal. We start with an obvious lemma.

Lemma 3.18 *If z and z_0 are complex numbers such that $\mathrm{Re}\,(z - z_0) > 0$, then*

$$
\frac{1}{z - z_0} = \int_0^\infty e^{-x(z-z_0)}\, dx.
\tag{99}
$$

16

Table 2: Quadrature nodes and weights for $N = 8$.

k	x_k	w_k
1	0.9743818326893713−01	0.2469944279808820+00
2	0.4917660712345750+00	0.5328649552527160+00
3	0.1147630094197554+01	0.7724853603957714+00
4	0.2028186101391804+01	0.9870187246041202+00
5	0.3121662089244688+01	0.1200121694721202+01
6	0.4425614160158614+01	0.1405423586612871+01
7	0.5925421085324173+01	0.1592796104486006+01
8	0.7601289009353128+01	0.1765198353876860+01

One of principal numerical tools of this paper is finite quadratures for the integrals of the form (99), approximating them by expressions of the form

$$\int_0^\infty e^{-x(z-z_0)} \, dx \sim \sum_{j=1}^N w_j e^{-x_j(z-z_0)}, \tag{100}$$

with w_j, x_j chosen to minimize the error of the approximation. It turns out that the classical Laguerre quadrature requires 56 nodes to obtain a full double precision (15-digit) approximation to (99) for all $z_0 \in \Omega_1^{in}$ and $z \in B_1$ (see Section 2.1 for the definition of B_1); it requires 28 nodes for single precision (7-digit) approximation and 14 nodes for the 3-digit approximation. In this paper, we use quadratures for integrals of the form (99) designed in [9]. The nodes and weights for the quadratures are listed in Tables 2–5 and the following lemma (proved in [9]) describes the performance of these quadratures when $z_0 \in \Omega_1^{in}$, $z \in B_1$.

Lemma 3.19 *1. If the nodes $x_1, x_2, \ldots, x_8$ and the weights $w_1, w_2, \ldots, w_8$ are those given in Table 2, then*

$$\left| \frac{1}{z - z_0} - \sum_{k=1}^8 w_k \, e^{-x_k(z-z_0)} \right| < 10^{-3} \tag{101}$$

for all $z_0 \in \Omega_1^{in}$, $z \in B_1$.
2. If the nodes $x_1, x_2, \ldots, x_{10}$ and the weights $w_1, w_2, \ldots, w_{10}$ are those given in Table 3, then

$$\left| \frac{1}{z - z_0} - \sum_{k=1}^{10} w_k \, e^{-x_k(z-z_0)} \right| < 10^{-4} \tag{102}$$

for all $z_0 \in \Omega_1^{in}$, $z \in B_1$.
3. If the nodes $x_1, x_2, \ldots, x_{16}$ and the weights $w_1, w_2, \ldots, w_{16}$ are those given in Table 4, then

$$\left| \frac{1}{z - z_0} - \sum_{k=1}^{16} w_k \, e^{-x_k(z-z_0)} \right| < 10^{-7} \tag{103}$$

17

Table 3: Quadrature nodes and weights for $N = 10$.

k	x_k	w_k
1	0.79400973700479499E–01	0.20213268247442060E+00
2	0.40599675027044617E+00	0.44529201310708538E+00
3	0.95860548270566906E+00	0.65492570079022383E+00
4	0.17076338623411169E+01	0.83991908942837771E+00
5	0.26342522431201576E+01	0.10125227869573986E+01
6	0.37330678114549477E+01	0.11856981580215332E+01
7	0.50056635563091912E+01	0.13587490932348730E+01
8	0.64476147019688304E+01	0.15237759923040743E+01
9	0.80499560865687445E+01	0.16815303253729583E+01
10	0.98062704155363723E+01	0.18393633495134454E+01

Table 4: Quadrature nodes and weights for $N = 16$.

k	x_k	w_k
1	0.50985651676060708E–01	0.13042997567403943E+00
2	0.26521044170119003E+00	0.29617079732513146E+00
3	0.63877523197814055E+00	0.44851876604376186E+00
4	0.11575210696261956E+01	0.58677848054269013E+00
5	0.18084194569861214E+01	0.71331490632911526E+00
6	0.25812535628463790E+01	0.83115583049433043E+00
7	0.34688375582342864E+01	0.94332332670457377E+00
8	0.44670816002182331E+01	0.10530465654290459E+01
9	0.55752269484049922E+01	0.11635980151835418E+01
10	0.67950948336753639E+01	0.12764875588622437E+01
11	0.81285324158592802E+01	0.13903417411114886E+01
12	0.95753440067592314E+01	0.15029785005709016E+01
13	0.11133967001554676E+02	0.16142090491898996E+01
14	0.12804196003878283E+02	0.17271419059134570E+01
15	0.14590645231278096E+02	0.18490423387442165E+01
16	0.16505707680646142E+02	0.19928836723099878E+01

Table 5: Quadrature nodes and weights for $N = 33$.

k	x_k	w_k
1	0.252222297727341369E−01	0.64680274571235485E−01
2	0.13247759128084677E+00	0.14962720607997425E+00
3	0.32380669248023823E+00	0.23260602282627724E+00
4	0.59671535823233030E+00	0.31267567589062277E+00
5	0.94802704428024797E+00	0.38936352755688915E+00
6	0.13742659894203061E+01	0.46253028974011126E+00
7	0.18719475451288249E+01	0.53228190405863132E+00
8	0.24377774897497581E+01	0.59887920022585347E+00
9	0.30687681826830449E+01	0.66266415869490855E+00
10	0.37622927481697938E+01	0.72400998959978491E+00
11	0.45161007854489040E+01	0.78329340463991183E+00
12	0.53283153101708052E+01	0.84088382086631104E+00
13	0.61974248981676391E+01	0.89714360915324316E+00
14	0.71222793332370721E+01	0.95243401551568258E+00
15	0.81020919953769825E+01	0.10071219382388539E+01
16	0.91364474341994351E+01	0.10615826335963539E+01
17	0.10225307113296538E+02	0.11161921501942585E+01
18	0.11368999161839711E+02	0.11713015487646939E+01
19	0.12568170717361438E+02	0.12271878679241548E+01
20	0.13823683086431786E+02	0.12839926657455333E+01
21	0.15136452987314821E+02	0.13416829044598757E+01
22	0.16507283044647311E+02	0.14000734153500639E+01
23	0.17936750445208845E+02	0.14589180106367176E+01
24	0.19425207754170005E+02	0.15180347903942609E+01
25	0.20972906955216222E+02	0.15774212769044868E+01
26	0.22580224099961821E+02	0.16373402708097615E+01
27	0.24247959886492881E+02	0.16983905310960812E+01
28	0.25977718733384464E+02	0.17616017849285610E+01
29	0.27772422510974588E+02	0.18286259025840425E+01
30	0.29637118447457170E+02	0.19021749030833896E+01
31	0.31580471971364523E+02	0.19870826536338642E+01
32	0.33617895925272799E+02	0.20930613125138042E+01
33	0.35778138778825402E+02	0.22428277080254514E+01

for all $z_0 \in \Omega_1^{in}$, $z \in B_1$.

4. If the nodes $x_1, x_2, \ldots, x_{33}$ and the weights $w_1, w_2, \ldots, w_{33}$ are those given in Table 5, then

$$\left| \frac{1}{z - z_0} - \sum_{k=1}^{33} w_k \, e^{-x_k(z-z_0)} \right| < 10^{-15} \tag{104}$$

for all $z_0 \in \Omega_1^{in}$, $z \in B_1$.

3.4 Informal Description

Obviously, approximating the integral (99) by a finite quadrature formula gives rise to an approximation of the function $\frac{1}{z-z_0}$ by a finite linear combination of exponentials in each of the regions Ω_1^{in}, B_1. Indeed, suppose that N_0 is a natural number, and positive real numbers $x_1, x_2, \ldots, x_{N_0}$, $w_1, w_2, \ldots, w_{N_0}$ are such that

$$\left| \int_0^\infty e^{-x(z-z_0)} \, dx - \sum_{k=1}^{N_0} w_k \, e^{-x_k(z-z_0)} \right| < \varepsilon, \tag{105}$$

for all $z_0 \in \Omega_1^{in}$, $z \in B_1$, and ε a sufficiently small positive number. Clearly, (105) can be rewritten in the form

$$\frac{1}{z - z_0} \sim \sum_{k=1}^{N_0} w_k \, e^{-x_k(z-z_0)}, \tag{106}$$

and, given an arbitrary point $w \in B_1$, (106) can be rewritten in the form

$$\frac{1}{z - z_0} \sim \sum_{k=1}^{N_0} w_k \, e^{-x_k(w-z_0)} \, e^{-x_k(z-w)}. \tag{107}$$

In other words, the potential of a charge at the point z_0 has been approximated by a linear combination of exponentials. For a potential Φ given by the formula

$$\Phi(z) = \sum_{i=1}^{m} \frac{q_i}{z - z_i} \tag{108}$$

due to a set of m charges of strengths $q_1, q_2, \ldots, q_m$ located at the points $z_1, z_2, \ldots, z_m$ in the square Ω_1^{in}, the expression (107) assumes the form

$$\Phi(z) = \sum_{i=1}^{m} \frac{q_i}{z - z_i} \sim \sum_{k=1}^{N_0} c_k \, e^{-x_k(z-w)}, \tag{109}$$

with the coefficients c_k defined by the formula

$$c_k = w_k \sum_{i=1}^{m} q_i \, e^{-x_k(w-z_i)}, \tag{110}$$

20

for all k $= 1,2,\ldots,N_0$. We will view (109) as an expansion of the function Φ into a linear combination of exponentials $e^{-x_k(z-w)}$, centered at w. Now, given another point $\tilde{w} \in B_1$, (109) assumes the form

$$\Phi(z) \sim \sum_{k=1}^{N_0} \tilde{c}_k \, e^{-x_k(z-\tilde{w})}, \tag{111}$$

and, obviously,

$$\tilde{c}_k = c_k \, e^{-x_k(\tilde{w}-w)}, \tag{112}$$

for all k $= 1,2,\ldots$. Thus, we are lead to the following observation.

Observation 3.20 *An expression of the form (111) represents the potential of an arbitrary combination of charges located in the region Ω_1^{in}, and the representation is valid for all $z \in B_1$. Furthermore, (112) can be interpreted to mean that in the representation (111), the translation operator for the potential fields is diagonal. In the following subsection we formalize this observation.*

3.5   Detailed Description

In this section, we use Lemma 3.19 to obtain exponential representations of the form (111) for potentials generated by collections of charges located in Ω_s^{in} at all scales $s > 0$. Error estimates for such representations are provided by Theorem 3.21 below. We start with the following obvious generalization of Lemma 3.19.

Theorem 3.21 *Suppose that $\varepsilon > 0$ is a real number, and real numbers $x_1, x_2, \ldots, x_{N_0}$ and $w_1, w_2, \ldots, w_{N_0}$ are such that*

$$\left| \frac{1}{z - z_0} - \sum_{n=1}^{N_0} w_n \, e^{-x_n(z-z_0)} \right| < \varepsilon \tag{113}$$

for all $z_0 \in \Omega_1^{in}$, $z \in B_1$. Suppose further that $s > 0$ is a real number, $w \in B_s$, and the functions $E_{n,s,w} : \mathbb{C} \to \mathbb{C}$ (n=1,2,\ldots,N_0), are defined by the formula

$$E_{n,s,w}(z) = \frac{1}{s} \, \exp(-x_n \frac{z-w}{s}), \tag{114}$$

for all $z \in \mathbb{C}$. Finally, suppose that

$$\Phi(z) = \sum_{i=1}^{m} \frac{q_i}{z_i - z} \tag{115}$$

is the potential due to a set of m charges of strengths $q_1, q_2, \ldots, q_m$ located at points $z_1, z_2, \ldots, z_m$ inside the square Ω_s^{in}. Then for any $z \in B_s$

$$\left| \Phi(z) - \sum_{n=1}^{N_0} b_n E_{n,s,w}(z) \right| < \frac{\varepsilon}{s} \sum_{i=1}^{m} |q_i|, \tag{116}$$

with

$$b_n = w_n \sum_{i=1}^{m} q_i \, \exp(-x_n \frac{w - z_i}{s}),$$
(117)

for all $n = 1,2,\dots,N_0$.

The following theorem is an immediate consequence of the definition (114) of the functions $E_{n,s,w}$.

Theorem 3.22 *Suppose that under the conditions of Theorem 3.21, $w, \tilde{w} \in B_s$ and*

$$\Phi(z) \sim \sum_{n=1}^{N_0} a_n E_{n,s,w}(z),$$
(118)

$$\Phi(z) \sim \sum_{n=1}^{N_0} b_n E_{n,s,\tilde{w}}(z),$$
(119)

are the expansions provided by Theorem 3.21. Then

$$b_n = \exp(-x_n \frac{\tilde{w} - w}{s}) \, a_n,$$
(120)

for all $n = 1,2,\dots,N_0$.

Suppose that $s > 0$ is a real number, $w \in B_s$ and $\Psi^{out}_{n,s,w}$, $E_{n,s,w}$ are functions defined by (58) and (114), respectively. We will define coefficients $r_{n,k,s,w}$ by the formula

$$r_{n,k,s,w} = \frac{w_n}{s_n} \int_{D_s^{in}} \overline{\Psi^{in}_{k,s,0}}(\xi) \, E_{n,s,\xi}(w) \, ds(\xi),$$
(121)

where $s_1, s_2, \dots,$ are given by (37) and k = 1,2,..., and n = 1,2,..., N_0.

Theorem 3.23 *Suppose that $s > 0$ is a real number, Φ given by the formula (63) is the potential due to a set of m charges of strengths $q_1, q_2, \dots, q_m$ located in the square Ω_s^{in}, and*

$$\Phi(z) = \sum_{n=1}^{\infty} a_n \Psi^{out}_{n,s,0}(z),$$
(122)

is the expansion provided by Theorem 3.8. Suppose further, that $\varepsilon > 0$ is a real number and

$$\Phi(z) \sim \sum_{n=1}^{N_0} b_n E_{n,s,w}(z),$$
(123)

is the approximation provided by Theorem 3.21. Then for $n = 1,2,\dots,N_0$

$$b_n = \sum_{k=1}^{\infty} r_{n,k,s,w} \, a_k,$$
(124)

with $r_{n,k,s,w}$ defined by (121).

22

Proof. Due to (58), Theorem 3.1 and Theorem 3.21

$$
\begin{aligned}
\Psi_{k,s,0}^{out}(z) &= \frac{1}{\sqrt{s}}\,\Psi_k^{out}\left(\frac{z}{s}\right) = \frac{1}{\sqrt{s}}s_k^{-1}\mathcal{C}_{out}\,\overline{\Psi_k^{in}}\left(\frac{z}{s}\right) \\
&= \frac{1}{\sqrt{s}}s_k^{-1}\int_{D_1^{in}}\frac{1}{\xi-\frac{z}{s}}\,\overline{\Psi_k^{in}}(\xi)ds(\xi) \\
&\sim \frac{1}{\sqrt{s}}\,s_k^{-1}\sum_{n=1}^{N_0}w_n\int_{D_1^{in}}e^{-x_n\left(\frac{z}{s}-\xi\right)}\,\overline{\Psi_k^{in}}(\xi)ds(\xi) \\
&= \frac{1}{\sqrt{s}}\,s_k^{-1}\sum_{n=1}^{N_0}w_n e^{-x_n\left(\frac{z-w}{s}\right)}\int_{D_s^{in}}s^{-1}e^{-x_n\left(\frac{w-\xi}{s}\right)}\,\overline{\Psi_k^{in}}\left(\frac{\xi}{s}\right)ds(\xi) \\
&= \sum_{n=1}^{N_0}r_{n,k,s,w}E_{n,s,w}(z),
\end{aligned}
\tag{125}
$$

for each $k = 1, 2, \ldots$. Now (124) follows immediately from (125). $\qquad\square$

Suppose that $s > 0$ is a real number, $w \in B_s$ and $\Psi_{n,s,w}^{out}$, $E_{n,s,w}$ are functions defined by (58) and (114), respectively. We will define coefficients $e_{n,k,s,w}$ by the formula

$$
e_{n,k,s,w} = \int_{D_s^{in}}\overline{\Psi_{k,s,0}^{in}}(\xi)\,E_{n,s,w}(\xi)\,ds(\xi),
\tag{126}
$$

$k = 1,2,\ldots$, and $n = 1,2,\ldots, N_0$.

The proof of the following theorem is quite similar to that of Theorem 3.8, and is omitted.

Theorem 3.24 *Suppose that $s > 0$ is a real number, Φ given by the formula (63) is the potential due to a set of m charges of strengths $q_1, q_2, \ldots, q_m$ located in the square Ω_s^{in}, and*

$$
\Phi(z) = \sum_{k=1}^{\infty}b_k\Psi_{k,s,0}^{in}(z),
\tag{127}
$$

is the expansion provided by Theorem 3.9. Suppose further, that $\varepsilon > 0$ is a real number and

$$
\Phi(z) \sim \sum_{n=1}^{N_0}a_n E_{n,s,w}(z),
\tag{128}
$$

is the approximation provided by Theorem 3.21. Then fork = 1,2,...

$$
b_k = \sum_{n=1}^{N_0}e_{n,k,s,w}\,a_n,
\tag{129}
$$

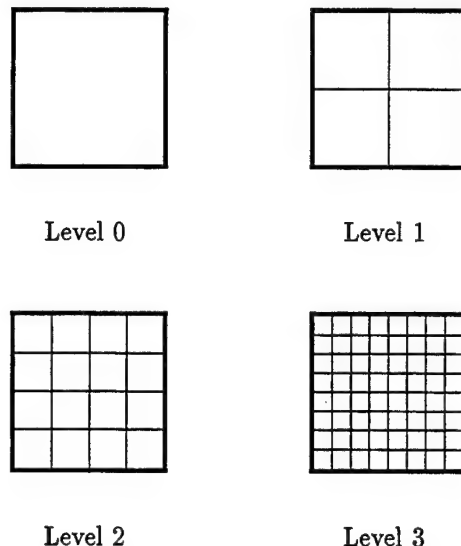*with $e_{n,k,s,w}$ defined by (126).*

23

Figure 3: The computational box and three levels of refinement.

4   The multipole algorithm

4.1   Notation

Without a loss of generality we can assume that all particles are located in the unit square centered at the origin. We will refer to this square as the computational box. A hierarchy of meshes is introduced in the computational box. Mesh level 0, denoted by B_0, corresponds to the entire computational box. Mesh level $l + 1$, denoted by B_{l+1}, is obtained from mesh level l by subdividing some boxes into four equal squares (see Figure 3), which will be referred to as children of the given square. We fix an integer number $s > 0$ and at each level we subdivide only those boxes, which contain more than s particles. A box which is not subdivided is called *childless*.

Colleagues of a box are adjacent boxes of the same size.

Two boxes of the same size which are not adjacent, are called *separated*.

For each box b there are four lists of other boxes, defined as follows.

List 1 of a box b is denoted by U_b; if b is childless, it consists of b and all childless boxes adjacent to b. If b is a parent box, then U_b is empty.

List 2 of a box b is denoted by V_b. V_b is formed by all the children of the colleagues of b's parent which are separated from b (see Figure 4).

List 3 of a box b is denoted by W_b. If b is childless, W_b consists of all descendants of

Figure 4: Interaction List 2 for a dashed box.

b's colleagues whose parents are adjacent to b, but which are not adjacent to b themselves. If b is a parent box, W_b is empty.

List 4 of a box b is denoted by X_b; it consists of all boxes b' such that $b' \in W_b$.

Ψ_b^{out} will denote the p-term expansion of the form (64) of the potential due to particles located in b.

Ψ_b^{in} will denote the p-term expansion of the form (64) of the potential due to particles located outside $U_b \cup W_b$.

4.2 Informal description of the algorithm

The data structure used by our algorithm is virtually identical to the one presented in [2]. It relies on clustering of particles at various scales. The computation of interactions between clusters separated from each other is performed via the expansions (64) and (67), while the interactions between nearby particles are computed directly.

In order to adapt our grid to a given distribution of particles we fix an integer $s > 0$ and subdivide only those boxes which contain more than s particles.

The algorithm consists of the following stages.

(1) We create a hierarchy of meshes in a computational cell.

(2) For each childless box b we directly evaluate interactions between particles in b and particles in U_b, List 1 of b.

(3) For each childless box b we form the expansion Ψ_b^{out} into outgoing singular functions by means of Theorem 3.8.
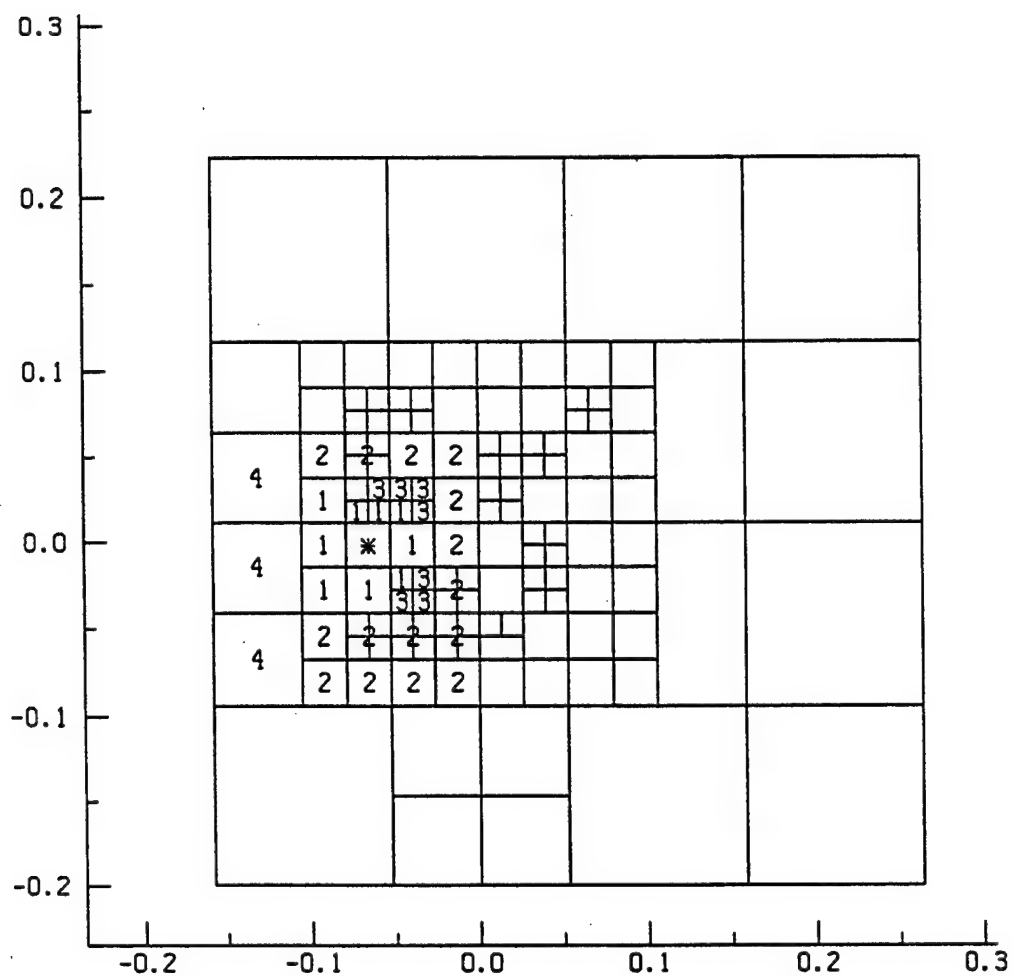
25

Figure 5: A box and associated Lists 1–4.

(4) For each parent box b we form the expansion Ψ_b^{out} by merging expansions of its children via Theorem 3.12.

(5) We convert all expansions Ψ_b^{out} into the exponential form via Theorem 3.23.

(6) We use Theorem 3.22 to shift the q-term exponential expansion to each box in V_b, List 2 of b.

(7) For every particle $r \in b$, we compute the field due to all particles in W_b, List 3 of b, by summing up the expansions Ψ_w^{out} for all $w \in W_b$ and add it to the potential at this point calculated in (1).

(8) We convert the field of each particle in X_b, List 4 of b, into the expansion Ψ_b^{in}.

(9) We convert all exponential expansions into expansions Ψ_b^{in} via Theorem 3.24 and combine them with the result of (8).

(10) For each child box b we shift the expansion of its parent (Theorem 3.9) and add it to the expansion Ψ_b^{in}.

(11) For each childless box b we evaluate the expansion Ψ_b^{in} at every particle $r \in b$ and add it to the result of (7), obtaining the field at r.

4.3   Detailed description of the algorithm

ALGORITHM

Comment [Choose main parameters.]

Choose precision ε to be achieved. Set the length of expansions according to Table 1.

Set the maximum number s of particles in a childless box.

Step 1

Comment [Refine a computational cell into a hierarchy of meshes.]

```
do l = 1,2,...
      do b_i ∈ B_l
            if b_i contains more than s particles then
                  subdivide b_i into four boxes and add the nonempty boxes
                  formed to B_{l+1}.
            end if
      end do
end do
```

Comment [We denote by *nlev* the highest level of refinement and by *nbox* the total number of boxes formed at Step 1.]

Step 2

Comment [For every particle in each childless box b compute directly the interactions with particles in U_b, List 1 of b.]

do i = 1,nbox
    if b_i is a childless box **then**
        for each particle $r \in b_i$ compute interactions between r and
        all particles in U_{b_i}.
    end if
end do

Step 3

Comment [For every childless box b form an expansion into outgoing singular functions about the center of b via Theorem 3.8.]

do i = 1,nbox
    if b_i is a childless box **then**
        use Theorem 3.7 to form a p-term expansion $\Psi_{b_i}^{out}$
        representing the potential due to all charges in b_i.
    end if
end do

Step 4

Comment [For each parent box b use Theorem 3.10 to shift the center of each b's child box's expansion to b's center and add the resulting expansions together.]

do l = nlev-1,1,-1
    do $b_i \in B_l$
        if b_i is a parent box **then**
            use Theorem 3.10 to obtain a p-term expansion $\Psi_{b_i}^{out}$ by
            shifting expansions of B_i's children to b and adding the
            resulting expansions together.
        end if
    end do
end do

Step 5

28

Comment [For each box b use Theorem 3.23 to convert the expansion Ψ_b^{out} to the
exponential form.]

do i = 1,nbox
use Theorem 3.23 to convert the expansion $\Psi_{b_i}^{out}$ to the exponential form.
end do

Step 6

Comment [For each box b use Theorem 3.22 to shift the exponential expansion from
b to each box in V_b, List 2 of b.]

do i = 1,nbox
use Theorem 3.22 to shift the exponential expansion from b to each box
in V_b, List 2 of b.
end do

Step 7

Comment [For each childless box b, evaluate the expansions Ψ_w^{out} for all $w \in W_b$,
List 3 of b, at every particle $r \in b$.]

do i = 1,nbox
if b is childless **then**
evaluate the expansion Ψ_w^{out} of each box $w \in W_b$ at every particle
$r \in b$.
end if
end do

Step 8

Comment [For each box b, create the expansion Ψ_b^{in} representing in b the field due to
particles in X_b, List 4 of b.]

do i = 1,nbox
Create the expansion Ψ_b^{in} of the field due to all particles in X_b.
end do

Step 9

Comment [For each box b use Theorem 3.24 to convert the exponential expansion
into the expansion of the form (67) and combine with the expansion Ψ_b^{in}

29

computed in Step 7.]

do i = 1,nbox

    use Theorem 3.24 to convert the exponential expansion the expansion of
the form (67) and computed it with the expansion $\Psi_{b_i}^{out}$.

end do

<div align="center">

Step 10

</div>

Comment [Use Theorem 3.12 to shift the local expansions Ψ^{in} of parent boxes to
their children.]

do l = 1,nlev-1

    do $b_i \in B_l$

        if b_i is a child box **then**

            use Theorem 3.12 to shift a p-term expansion Ψ^{in}
from b's parent to b and update Ψ_b^{in}.

        end if

    end do

end do

<div align="center">

Step 11

</div>

Comment [For every childless box b evaluate the expansion Ψ_b^{in} at each particle
$r \in b$ and add it to the result of Step 7, obtaining the potential at r.]

do i = 1,nbox

    if b_i is childless **then**

        for each particle $r \in b_i$ evaluate the p-term expansion $\Psi_{b_i}^{in}$
obtaining the potential at location r.

    end if

end do

4.4 Complexity analysis

Step Operation
       count

Step	count	
1	Np	Each particle is assigned to a box at every level. There are at most p levels of refinement.
2	33Nps	The direct computation of interactions between any two

<div align="center">

30

</div>

		childless boxes requires at most $\frac{3s^2}{2}$ operations. The total number of boxes appearing on a List 1 of a box does not exceed $\frac{44Np}{s}$ (see [2]).
3	Np	Each particle contributes to a p-term expansion Ψ_b^{out} of a unique childless box b containing it.
4	$\frac{5Np^3}{s}$	Each translation requires p^2 operations and there are at most $\frac{5Np}{s}$ boxes (see [2]).
5	$\frac{5Np^2q}{s}$	Each translation requires pq operations. The total number of boxes is bounded by $\frac{5Np}{s}$.
6	$\frac{135Npq}{s}$	Each diagonal translation requires q operations and there are at most 27 boxes on any List 2.
7	$32Np^2$	Computing the interactions of all particles in a box b with a box in W_b requires ps operations. The total number of boxes appearing on a List 3 does not exceed $\frac{32Np}{s}$ (see [2]).
8	$32Np^2$	Computing the interactions of a box b with all particles in a box in X_b requires ps operations. The total number of boxes appearing on a List 4 does not exceed $\frac{32Np}{s}$ (see [2]).
9	$\frac{5Np^2q}{s}$	Each translation requires pq operations. The total number of boxes is bounded by $\frac{5Np}{s}$.
10	$\frac{5Np^3}{s}$	Each translation requires p^2 operations.
11	$Np+N$	A p-term expansion Ψ_b^{out} is evaluated at each particle. Summing up requires extra N operations.

Combining the CPU times for all the above stages, we obtain the estimate

$$T = N(a\,\frac{p^3}{s} + b\,\frac{p^2q}{s} + cps + dp^2), \qquad (130)$$

where the constants a, b, c, d depend on the implementation. The parameter s, the maximum number of particles in a childless box, should be chosen so as to minimize the CPU time. An elementary calculation shows that the minimal time T_{min}

$$T_{min} = Np^2\sqrt{\alpha + \beta\,\frac{q}{p}}, \qquad (131)$$

is obtained for

$$s_{min} = \frac{p}{\sqrt{c}}\sqrt{a + b\,\frac{q}{p}}, \qquad (132)$$

31

with constants α, β dependent on the particular implementation. Since $p \sim q$, we arrive at the estimate

$$T_{min} = \gamma N p^2 = \gamma N \, (\log_2 \frac{1}{\varepsilon})^2, \tag{133}$$

where the constant γ depends on the implementation.

The storage requirements are determined by the lentgh of expansions and the total number of boxes, which does not exceed $\frac{5Np}{s}$. Per box, we store $2p$ coefficients of singular functions and $4q$ coefficients of exponentials. Additionally, we store the position and the charge of each particle and corresponding p values of singular functions. Therefore, the storage requirements are of the form

$$S = N(c_1 \, \frac{10p^2 + 20pq}{s} + c_2 p) \tag{134}$$

with the constants c_1, c_2 dependent on the implementation. If $s = s_{min}$, we obtain

$$S = c_3 \, N \log_2 \frac{1}{\varepsilon}, \tag{135}$$

where c_3 depends on the implementation.

Remark 4.1 A careful examination of (135) shows that even though the storage requirements of the algorithm are proportional to the number of particles, the associated constant is quite large, especially in double precision calclations. This limits the size of problems which can be handled in computing environments where the available memory is limited. Moreover in systems with virtual memory, it is liable to increase the wall-clock time of the algorithm. This problem is presently being addressed by the authors.

5 Numerical results

The algorithm described in Section 4 has been implemented in Fortran 77 and numerical experiments have been performed on a SPARCstation 2. We compare its performance with an implementation of the FMM from [2], and with direct application of the potential matrix. We give the results for three regimes: particles uniformly distributed in a square, particles located uniformly on a curve and particles clustered within a square. All calculations were done in double precision, and extended (quadruple) precision was used to determine the relative errors. The number of particles varied between 400 and 25,600, with charge strengths randomly distributed on the interval $(0, 1)$.

The results of our experiments are given in Tables (6–8). In each table the first column contains the number N of particles in a simulation. Second,third and forth columns show the CPU times $T_{new}, T_{old}, T_{dir}$ in seconds of the present algorithm, the algorithm described in [2] and of the direct calculation, respectively. The fifth, the sixth

Table 6: Uniformly distributed particles.

N	T_{new}	T_{old}	T_{dir}	E_{new}	E_{old}	E_{dir}
400	0.3	1.5	1.0	$2.2\,10^{-16}$	$4.4\,10^{-16}$	$4.3\,10^{-16}$
800	0.8	2.7	4.1	$3.4\,10^{-16}$	$1.4\,10^{-15}$	$6.1\,10^{-16}$
1600	1.5	7.1	16.9	$3.4\,10^{-16}$	$5.2\,10^{-15}$	$2.2\,10^{-16}$
3200	3.5	10.9	68.6	$3.1\,10^{-16}$	$1.3\,10^{-15}$	$8.5\,10^{-16}$
6400	6.4	32.2	277.3	$2.4\,10^{-16}$	$5.6\,10^{-16}$	$1.3\,10^{-15}$
12800	12.9	46.9	(1100)	$3.6\,10^{-16}$	$4.9\,10^{-16}$	—
25600	26.7	143.5	(4400)	$4.9\,10^{-16}$	$4.6\,10^{-16}$	—

Table 7: Particles distributed on a curve.

N	T_{new}	T_{old}	T_{dir}	E_{new}	E_{old}	E_{dir}
400	0.3	1.2	1.0	$2.6\,10^{-14}$	$1.7\,10^{-14}$	$2.5\,10^{-14}$
800	0.6	2.5	4.2	$2.3\,10^{-14}$	$3.2\,10^{-14}$	$2.3\,10^{-14}$
1600	1.2	3.8	17.2	$7.7\,10^{-14}$	$9.2\,10^{-14}$	$5.1\,10^{-14}$
3200	2.6	7.7	69.4	$3.4\,10^{-14}$	$4.1\,10^{-14}$	$8.9\,10^{-14}$
6400	5.4	15.4	283.2	$2.1\,10^{-13}$	$2.8\,10^{-13}$	$3.1\,10^{-13}$
12800	10.9	30.7	(1100)	$2.3\,10^{-13}$	$3.7\,10^{-13}$	—
25600	21.6	58.8	(4400)	$7.4\,10^{-13}$	$6.9\,10^{-13}$	—

and the seventh column contain the corresponding relative errors $E_{new}, E_{old}, E_{dir}$. The errors are computed in the l^2 norm via the formula

$$E = \frac{\left(\sum_{i=1}^{N} |\Phi_i - \tilde{\Phi}_i|^2\right)^{\frac{1}{2}}}{\left(\sum_{i=1}^{N} |\Phi_i|^2\right)^{\frac{1}{2}}}, \qquad (136)$$

where Φ_i is the value of the potential at the ith particle position obtained in a direct calculation in extended (quadruple) precision, and $\tilde{\Phi}_i$ is the corresponding value obtained by one of the three methods in question.

In the first set of experiments particle positions are generated randomly, resulting in their nearly uniform distribution (Figure 5). In the second set of tests particles are uniformly distributed on an ellips (Figure 6). The third set of tests is performed for a nonuniform distribution of particles within a square (Figure 7).

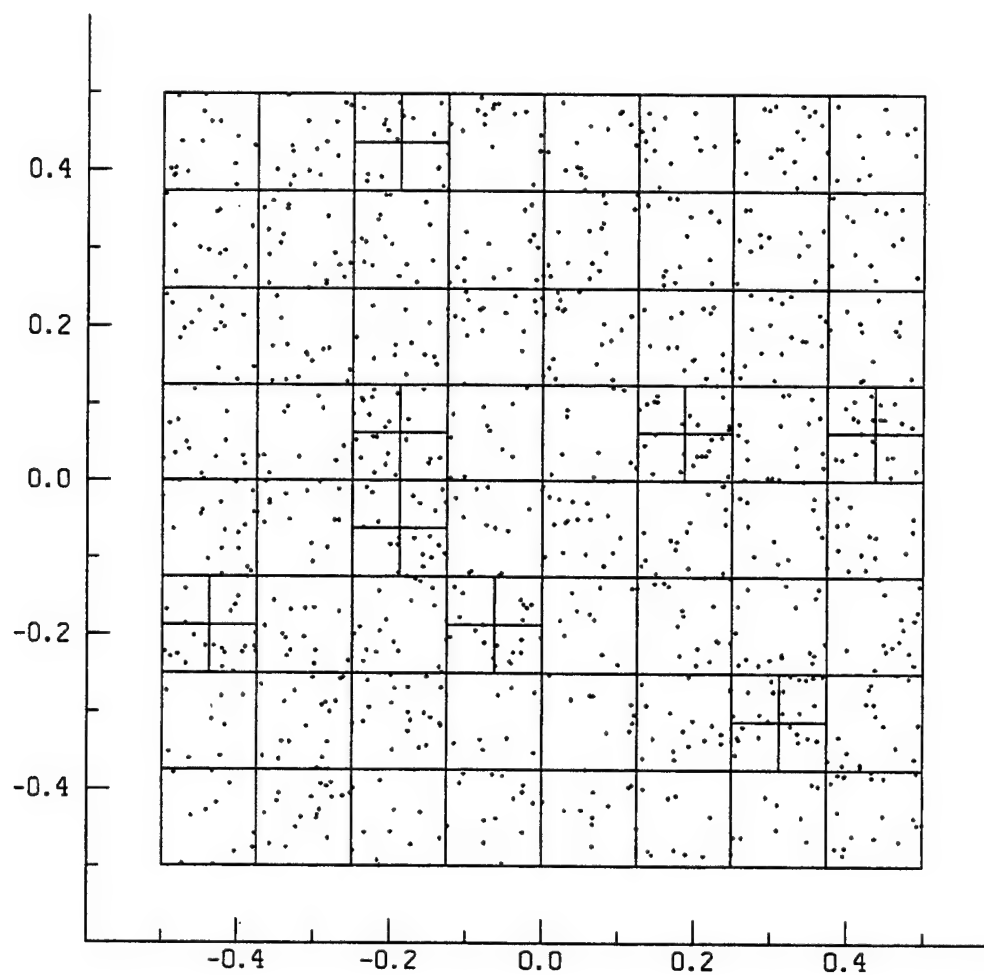In all cases the maxium number of particles in a childless box is set to 44.

Figure 6: Uniformly distributed particles and the associated partition of the computational box.
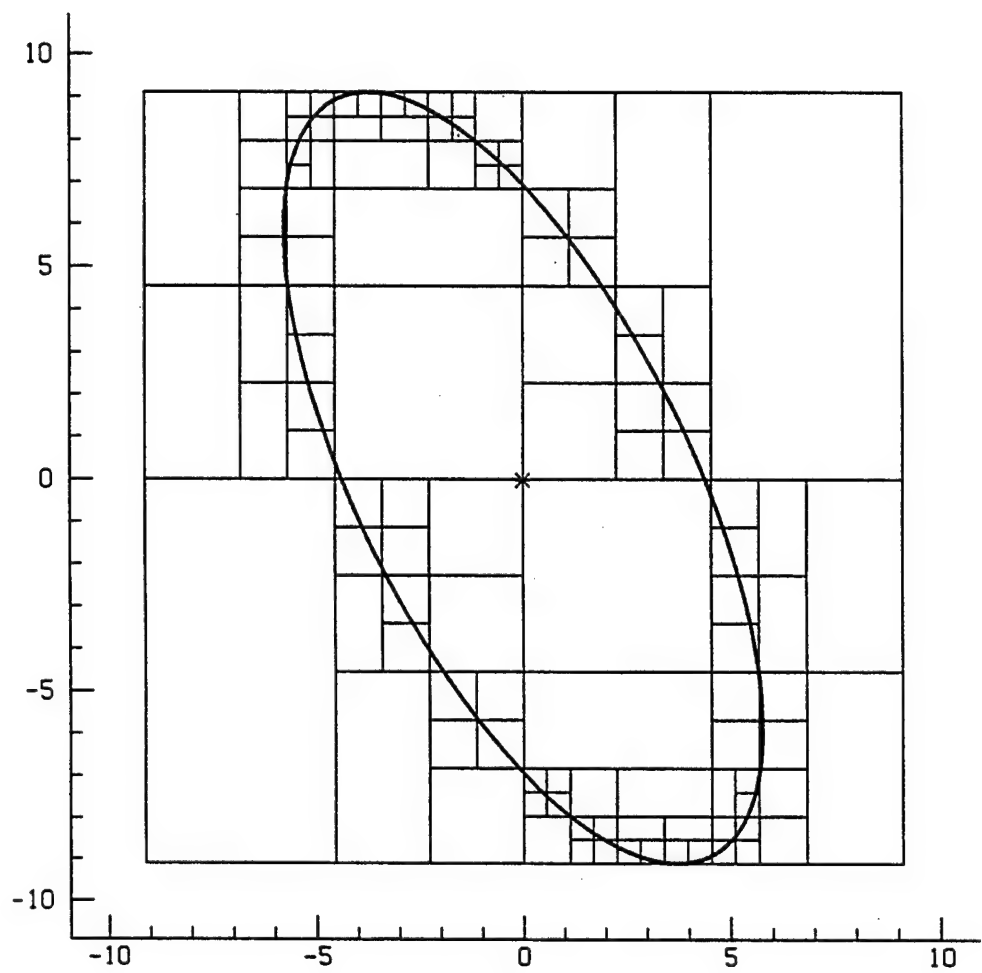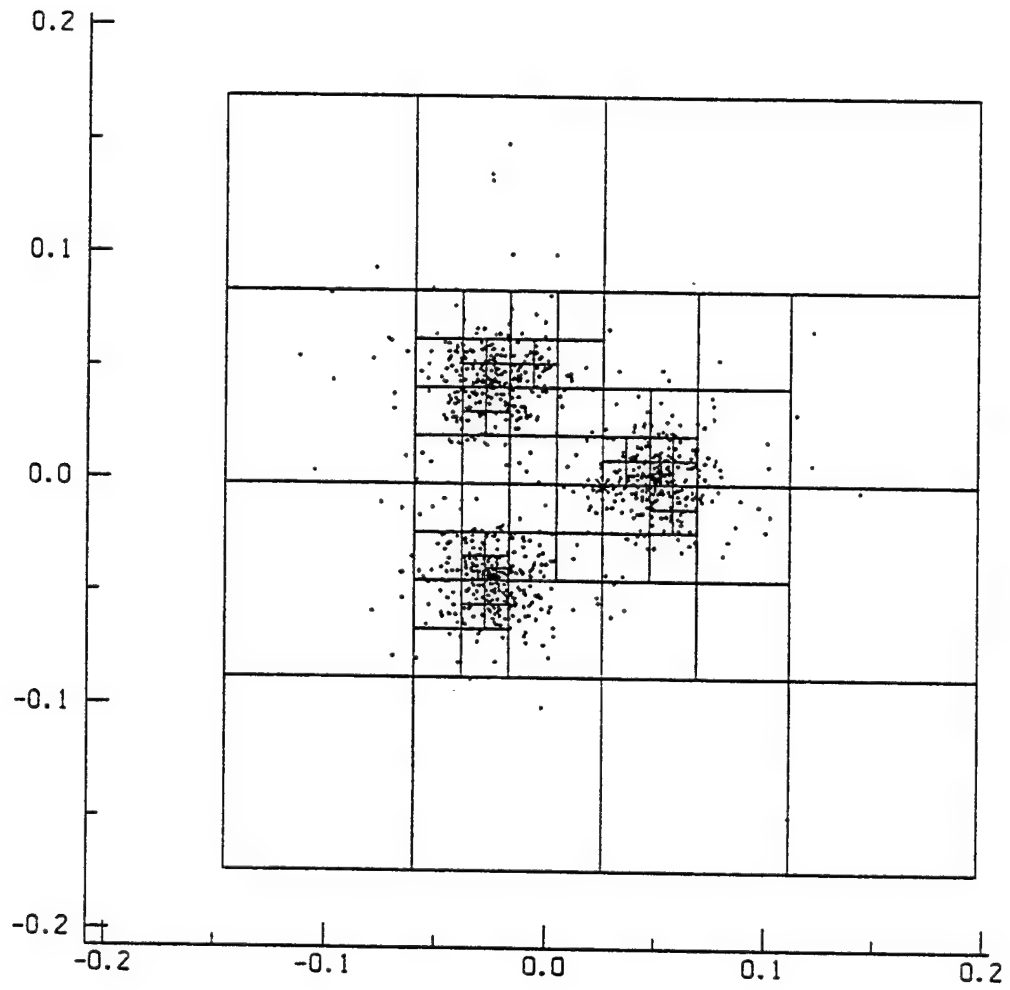
Figure 7: Particles distributed on a curve.

Figure 8: A nonuniform distribution of particles.

Table 8: A nonuniform distribution of particles.

N	T_{new}	T_{old}	T_{dir}	E_{new}	E_{old}	E_{dir}
400	0.5	1.4	1.0	$3.5\,10^{-13}$	$3.5\,10^{-13}$	$3.0\,10^{-13}$
800	1.2	2.8	4.2	$1.1\,10^{-12}$	$1.1\,10^{-12}$	$1.1\,10^{-12}$
1600	2.3	5.2	17.1	$1.1\,10^{-12}$	$1.1\,10^{-12}$	$1.1\,10^{-12}$
3200	4.9	11.6	69.0	$3.9\,10^{-13}$	$3.9\,10^{-13}$	$3.7\,10^{-13}$
6400	8.7	25.8	285.2	$4.9\,10^{-13}$	$4.9\,10^{-13}$	$2.7\,10^{-12}$
12800	17.8	52.6	(1100)	$6.7\,10^{-12}$	$6.8\,10^{-12}$	—
25600	34.7	110.6	(4400)	$2.5\,10^{-12}$	$2.5\,10^{-12}$	—

The following observations can be made from the experiments:

(1) The CPU time of the present algorithm grows linearly with N. The breakeven point with the direct calculation ranges from $N_0 = 140$ for uniformly distributed particles to $N_0 = 190$ for a highly nonuniform distribution.

(2) The performance of the algorithm does not depend significantly on the type of the particle distribution. The timings for a highly nonuniform distribution are about 60% higher that in the case of uniformly distributed particles.

(3) The accuracy obtained by the algorithm agrees with the error bounds (3.15) and (3.13).

6   Conclusions

A new version of the Fast Multipole algorithm for Coulombic interactions has been developed. While the prior schemes use Laurent and Taylor series to represent the potential, we use singular functions of an appropriately chosen operator, obtaining a much faster convergence. We also introduce an intermediate representation, in which most translation operators are diagonal. In two dimensions, the resulting scheme is three to five times faster than the best implementations of the old FMM we are aware of; we expect the ratio to be much higher in three dimensions.

The CPU time estimate and the storage requirements for the algorithm are of the order of $O(N)$, where N is the number of particles. Its performance does not depend significantly on the particle distribution.

The three-dimensional version of the algorithm is being implemented, and will be presented at a later date.

Appendix A

Estimates for the singular values of the operators $\mathcal{C}_{in}$ and $\mathcal{C}_{out}$

In this section we will express the operators $\mathcal{C}_{in} : L^2(D^{out}) \to L^2(D^{in})$, $\mathcal{C}_{out} : L^2(D^{in}) \to L^2(D^{out})$ by means of the Cauchy integral operator commonly encountered in complex analysis and derive inequalities (39) from corresponding inequalities for the new operator.

We will define arclength parametrizations $\gamma_1 : [0,4] \to D^{in}$, $\gamma_2 : [0,12] \to D^{out}$, of the squares D^{in}, D^{out}, respectively, by the formulas

$$
\gamma_1(t) = \begin{cases}
\frac{1}{2} - t + \frac{1}{2}i & \text{for} \quad 0 \le t \le 1 \\
-\frac{1}{2} + (\frac{1}{2} - t)i & \text{for} \quad 1 \le t < 2 \\
-\frac{1}{2} + t - \frac{1}{2}i & \text{for} \quad 2 \le t < 3 \\
\frac{1}{2} + (-\frac{1}{2} + t)i & \text{for} \quad 3 \le t < 4
\end{cases}
\tag{137}
$$

$$
\gamma_2(t) = 3\,\gamma_1\left(\frac{t}{3}\right) \qquad \text{for} \qquad 0 \le t \le 12.
\tag{138}
$$

Obviously, except for the corners of the squares, γ_1, γ_2 are differentiable and $|\gamma_1'| = |\gamma_2'| = 1$.

Finally, we define the Cauchy integral operator $\mathcal{C}_0 : L^2(D^{in}) \to L^2(D^{out})$ by the formula

$$
\begin{aligned}
\mathcal{C}_0 f(z) &= \frac{1}{2\pi i} \int_\gamma \frac{f(\xi)}{\xi - z}\, d\xi \\
&= \frac{1}{2\pi i} \int_{D^{in}} \frac{f(\xi)\gamma'(\xi)}{\xi - z}\, ds(\xi).
\end{aligned}
\tag{139}
$$

Observation A.1 *Denoting by* $M_{\gamma_1'} : L^2(D^{in}) \to L^2(D^{in})$ *the unitary operator of multiplication by* γ_1', *we observe that* $\mathcal{C}_0 = \mathcal{C}_{out} M_{\gamma_1'}$. *Therefore, the singular values of the operator* $\mathcal{C}_{out}$ *are identical to those of* $\mathcal{C}_0$.

Suppose that r_1, r_2 are real numbers such that $\frac{\sqrt{2}}{2} < r_1 < r_2 < \frac{3}{2}$. We will denote by S_1 and S_2 the circles $S_1 = \{|z| = r_1\}$ and $S_2 = \{|z| = r_2\}$ oriented counterclockwise. We define, respectively, the integral operators $\mathcal{C}_1^{r_2} : L^2(S_2) \to L^2(D^{out})$, $\mathcal{C}_2^{r_1,r_2} : L^2(S_1) \to L^2(S_2)$, $\mathcal{C}_3^{r_1} : L^2(D^{in}) \to L^2(S_1)$ by the formulae

$$
\mathcal{C}_1^{r_2} f(z) = \frac{1}{2\pi i} \int_{S_2} \frac{f(\xi)}{\xi - z}\, d\xi,
\tag{140}
$$

$$C_2^{r_1,r_2} f(z) = \frac{1}{2\pi i} \int_{S_1} \frac{f(\xi)}{\xi - z} \, d\xi, \tag{141}$$

$$C_3^{r_1} f(z) = \frac{1}{2\pi i} \int_{\gamma} \frac{f(\xi)}{\xi - z} \, d\xi. \tag{142}$$

Lemma A.2 *If the operators C_0, $C_1^{r_2}$, $C_2^{r_1,r_2}$, $C_3^{r_1}$ are defined by formulae (139-142), respectively, and $\frac{\sqrt{2}}{2} < r_1 < r_2 < \frac{3}{2}$, then*

$$C_0 = C_1^{r_2} C_2^{r_1,r_2} C_3^{r_1}. \tag{143}$$

Proof. Applying twice Cauchy's integral formula for an unbounded domain (see [6, vol.1, p.318]), for an arbitrary function $f \in L^2(D^{in})$ we have

$$C_2^{r_1,r_2}(C_3^{r_1} f)(\xi) = -C_3^{r_1} f(\xi), \qquad (\xi \in S_2), \tag{144}$$

$$C_1^{r_2}(C_3^{r_1} f)(z) = -C_3^{r_1} f(z), \qquad (z \in D^{out}). \tag{145}$$

Combining (144) with (145), we obtain

$$C_1^{r_2}(C_2^{r_1,r_2} C_3^{r_1} f)(z) = C_1^{r_2}(-C_3^{r_1} f)(z) = C_3^{r_1} f(z) = C_0 f(z), \tag{146}$$

for any $z \in D^{out}$. $\qquad \square$

The following lemma is well-known (see [3, p.98 and p.144]).

Lemma A.3 *Suppose that X_1, X_2, X_3, X_4, are piecewise smooth curves in $\mathbb{R}^2$. If $A : L^2(X_2) \to L^2(X_1)$, $B : L^2(X_3) \to L^2(X_2)$, $C : L^2(X_4) \to L^2(X_3)$ are bounded integral operators, and B is a Hilbert-Schmidt operator, then the composition ABC is a Hilbert-Schmidt operator. Moreover, if we denote by $s_n(B)$ and $s_n(ABC)$ the singular values of the operators B and ABC, respectively, then*

$$s_n(ABC) \leq \|A\| \, \|C\| \, s_n(B), \tag{147}$$

for all $n=1,2,\ldots$.

Lemma A.4 *Suppose, that $\{\phi_n\}$ and $\{\psi_n\}$ are orthonormal systems in $L^2(S_1)$ and $L^2(S_2)$, respectively defined for $n=1,2,\ldots$, by formulae*

$$\phi_n(\xi) = \frac{1}{\sqrt{2\pi r_1}} \left(\frac{r_1}{\xi} \right)^n, \tag{148}$$

$$\psi_n(z) = -\frac{1}{\sqrt{2\pi r_2}} \left(\frac{r_2}{z} \right)^n. \tag{149}$$

Then

$$C_2^{r_1,r_2} f = \sum_{n=1}^{\infty} \left(\frac{r_1}{r_2}\right)^{n-\frac{1}{2}} \langle f, \phi_n \rangle \, \psi_n, \tag{150}$$

is a Singular Value Decomposition for the operator $C_2^{r_1,r_2} : L^2(S_1) \to L^2(S_2)$. In particular, the singular values $s_n(C_2^{r_1,r_2})$ of $C_2^{r_1,r_2}$ are given by the formulae

$$s_n(C_2^{r_1,r_2}) = \left(\frac{r_1}{r_2}\right)^{n-\frac{1}{2}}, \tag{151}$$

for $n=1,2,\dots$.

Proof. Obviously, for any $\xi \in S_1$, $z \in S_2$,

$$\frac{1}{\xi - z} = -\sum_{n=1}^{\infty} z^{-n} \, \xi^{n-1}. \tag{152}$$

Combining (141) with (152), we obtain

$$
\begin{aligned}
C_2^{r_1,r_2} f(z) &= \frac{1}{2\pi i} \int_{S_1} \frac{f(\xi)}{\xi - z} \, d\xi = -\frac{1}{2\pi i} \sum_{n=1}^{\infty} z^{-n} \int_{S_1} f(\xi) \, \xi^{n-1} \, d\xi \\
&= -\frac{1}{2\pi r_1} \sum_{n=1}^{\infty} z^{-n} \int_{S_1} f(\xi) \, \xi^n \, ds(\xi) \\
&= \frac{1}{2\pi r_1} \sum_{n=1}^{\infty} \sqrt{2\pi r_2} \, r_2^{-n} \, \psi_n(z) \int_{S_1} f(\xi) \, \sqrt{2\pi r_1} \, r_1^n \, \overline{\phi_n(\xi)} \, ds(\xi) \\
&= \sum_{n=1}^{\infty} \left(\frac{r_1}{r_2}\right)^{n-\frac{1}{2}} \langle f, \phi_n \rangle \, \psi_n(z).
\end{aligned} \tag{153}
$$

$\square$

The following two theorems establish bounds from above and from below for the singular values of the operator C_{out}. We only prove Theorem A.5 below; the proof of Theorem A.6 is nearly identical, and is omitted.

Theorem A.5 *For any real number $\frac{\sqrt{2}}{3} < \rho < 1$ there exists a constant $c > 0$, such that*

$$s_n(C_{out}) \le c\rho^n, \tag{154}$$

for all $n=1,2,\dots$, where $s_n(C_{out})$ are the singular values of the operator C_{out}.

Proof. Defining real numbers r_1, r_2 by the formulae

$$r_1 = \frac{\sqrt{2} + 3\rho}{4}, \tag{155}$$

40

$$r_2 = \frac{r_1}{\rho}, \tag{156}$$

we observe that

$$\frac{\sqrt{2}}{2} < r_1 < r_2 < \frac{3}{2}. \tag{157}$$

Let us consider the operators $\mathcal{C}_0$, $\mathcal{C}_1^{r_2}$, $\mathcal{C}_2^{r_1,r_2}$, $\mathcal{C}_3^{r_1}$ defined by formulae (139–142). Clearly, $\frac{\sqrt{2}}{2} < r_1 < r_2 < \frac{3}{2}$. $\rho = \frac{r_1}{r_2}$. Combining (143) with (147), we obtain

$$s_n(\mathcal{C}_0) = s_n(\mathcal{C}_1^{r_2} \mathcal{C}_2^{r_1,r_2} \mathcal{C}_3^{r_1}) \leq \|\mathcal{C}_1^{r_2}\| \, s_n(\mathcal{C}_2^{r_1,r_2}) \, \|\mathcal{C}_3^{r_1}\|. \tag{158}$$

According to Observation A.1, the singular values of operators $\mathcal{C}_{out}$ and $\mathcal{C}_0$ coincide. Now Lemma A.4 gives

$$s_n(\mathcal{C}_{out}) = s_n(\mathcal{C}_0) \leq \|\mathcal{C}_1^{r_2}\| \, s_n(\mathcal{C}_2^{r_1,r_2}) \, \|\mathcal{C}_3^{r_1}\| = c \left(\frac{r_1}{r_2} \right)^n = c\rho^n, \tag{159}$$

for all n=1,2,.... $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ $\square$

Theorem A.6 *For any number $0 < \rho < \frac{1}{3\sqrt{2}}$ there exists a constant $c > 0$, such that*

$$s_n(\mathcal{C}_{out}) \geq c\rho^n, \tag{160}$$

for all n=1,2,..., where $s_n(\mathcal{C}_{out})$ denote the singular values of the operator $\mathcal{C}_{out}$.

Appendix B

Estimates for the singular functions of the operators $\mathcal{C}_{in}$ and $\mathcal{C}_{out}$

In this section we estimate the maxima of singular functions of the operator $\mathcal{C}_{out}$. We begin with four technical lemmas.

Lemma B.1 *If $n > 0$ is an integer and $P : \mathbb{C} \to \mathbb{C}$ is a polynomial of degree $n-1$, then*

$$\|P\|_{L^\infty[-1,1]} \leq \frac{n}{\sqrt{2}} \, \|P\|_{L^2[-1,1]}, \tag{161}$$

(for definitions of $\|\cdot\|_{L^2[-1,1]}$ and $\|\cdot\|_{L^\infty[-1,1]}$ see Section 2.1).

Proof. Let P_k denote the Legendre polynomials on the segment $[-1,1]$. It is well-known (see [1]), that

$$\|P_k\|_{L^\infty[-1,1]} = 1, \tag{162}$$

$$\|P_k\|^2_{L^2[-1,1]} = \frac{2}{2k+1}. \tag{163}$$

Obviously, there exist unique complex coefficients $c_0, c_1, \ldots, c_{n-1}$ such that

$$P = \sum_{k=0}^{n-1} c_k \, P_k, \tag{164}$$

and, consequently,

$$\|P\|^2_{L^2[-1,1]} = \sum_{k=0}^{n-1} |c_k|^2 \, \|P_k\|^2_{L^2[-1,1]} = \sum_{k=0}^{n-1} |c_k|^2 \, \frac{2}{2k+1}. \tag{165}$$

Now, due to Schwarz's inequality, we have

$$
\begin{aligned}
\|P\|_{L^\infty[-1,1]} &\leq \sum_{k=0}^{n-1} |c_k| \, \|P_k\|_{L^\infty[-1,1]} = \sum_{k=0}^{n-1} |c_k| = \sum_{k=0}^{n-1} \frac{\sqrt{2k+1}}{\sqrt{2}} \, |c_k| \, \frac{\sqrt{2}}{\sqrt{2k+1}} \\
&\leq \left(\sum_{k=0}^{n-1} \frac{2k+1}{2} \right)^{\frac{1}{2}} \left(\sum_{k=0}^{n-1} |c_k|^2 \frac{2}{2k+1} \right)^{\frac{1}{2}} = \frac{n}{\sqrt{2}} \, \|P\|_{L^2[-1,1]}.
\end{aligned} \tag{166}
$$

$\square$

The following lemma is readily obtained from Lemma B.1 by scaling.

42

Lemma B.2 *Suppose, that $n > 0$ is an integer and $P : \mathbb{C} \to \mathbb{C}$ is a polynomial of degree $n - 1$. If $I \subset \mathbb{C}$ is any segment of length $a > 0$, then*

$$\|P\|_{L^\infty(I)} \leq \frac{n}{\sqrt{a}} \|P\|_{L^2(I)}. \tag{167}$$

Lemma B.3 *There exists a constant $c_1 > 0$ such that for any segment $I \subset D^{out}$ of length $a > 0$, integer $n > 0$ and any $f \in L^2(D^{in})$ there exists a polynomial P of degree $n - 1$ satisfying*

$$\|\mathcal{C}_{out}f - P\|_{L^\infty(I)} \leq c_1 \, a^n \, \|f\|_2, \tag{168}$$

with the operator $\mathcal{C}_{out} : L^2(D^{in}) \to L^2(D^{out})$ defined by (30).

Proof. Differentiating (30) n times we obtain

$$(\mathcal{C}_{out}f)^{(n)}(z) = n! \int_{D^{in}} \frac{f(\xi)}{(\xi - z)^{(n+1)}} \, ds(\xi), \tag{169}$$

and, due to Schwarz's inequality, we have

$$\|(\mathcal{C}_{out}f)^{(n)}\|_\infty \leq c_1 \, n! \, \|f\|_2, \tag{170}$$

where $c_1 > 0$ is a constant. Let us denote by z_0 the midpoint of the segment I and let P be the Taylor polynomial of order $n - 1$ centered at z_0 for the function $\mathcal{C}_{out}f$. Now, the Taylor's formula implies that

$$|\mathcal{C}_{out}f(z) - P(z)| \leq \frac{|z - z_0|^n}{n!} \max_{\zeta \in I} |(\mathcal{C}_{out}f)^{(n)}(\zeta)|, \tag{171}$$

and therefore

$$\|\mathcal{C}_{out}f - P\|_{L^\infty(I)} \leq \frac{a^n}{2^n \, n!} \|(\mathcal{C}_{out}f)^{(n)}\|_\infty \leq c_1 \frac{a^n}{2^n} \|f\|_2 \leq c_1 \, a^n \, \|f\|_2. \tag{172}$$

$\square$

Lemma B.4 *There exists a constant $c > 0$, such that for any $f \in L^2(D^{in})$*

$$\|\mathcal{C}_{out}f\|_\infty \leq c \, \|\mathcal{C}_{out}f\|_2 \left(\log \frac{\|\mathcal{C}_{out}\|\|f\|_2}{\|\mathcal{C}_{out}f\|_2} + 1 \right), \tag{173}$$

where the operator $\mathcal{C}_{out} : L^2(D^{in}) \to L^2(D^{out})$ is defined by (30).

43

Proof. Let $0 < a < 1$ be a real number and I any segment of length a included in the square D^{out}. For an integer $n > 0$ and $f \in L^2(D^{in})$ denote by P the polynomial provided by Lemma A.9. Due to Lemma A.8 we have

$$
\begin{aligned}
\|\mathcal{C}_{out}f\|_{L^\infty(I)} &\leq \|\mathcal{C}_{out}f - P\|_{L^\infty(I)} + \|P\|_{L^\infty(I)} \\
&\leq \|\mathcal{C}_{out}f - P\|_{L^\infty(I)} + \frac{n}{\sqrt{a}}\|P\|_{L^2(I)}.
\end{aligned}
\tag{174}
$$

We will need the following obvious inequality

$$
\begin{aligned}
\|P\|_{L^2(I)} &\leq \|\mathcal{C}_{out}f - P\|_{L^2(I)} + \|\mathcal{C}_{out}f\|_{L^2(I)} \\
&\leq \sqrt{a}\,\|\mathcal{C}_{out}f - P\|_{L^\infty(I)} + \|\mathcal{C}_{out}f\|_{L^2(I)}.
\end{aligned}
\tag{175}
$$

Combining (168), (174) and (175) we obtain

$$
\begin{aligned}
\|\mathcal{C}_{out}f\|_{L^\infty(I)} &\leq (n+1)\,\|\mathcal{C}_{out}f - P\|_{L^\infty(I)} + \frac{n}{\sqrt{a}}\|\mathcal{C}_{out}f\|_{L^2(I)} \\
&\leq c_2\, n\left(a^n\|f\|_2 + \frac{1}{\sqrt{a}}\|\mathcal{C}_{out}f\|_2\right) \\
&\leq c_3\, n\,\|\mathcal{C}_{out}f\|_2\left(a^n\frac{\|\mathcal{C}_{out}\|\|f\|_2}{\|\mathcal{C}_{out}f\|_2} + \frac{1}{\sqrt{a}}\right),
\end{aligned}
\tag{176}
$$

with some constants $c_2 > 0$, $c_3 > 0$. Setting $a = \frac{1}{e}$ (where e is the base of natural logarithms), and

$$
n = \left\lfloor \log\frac{\|\mathcal{C}_{out}\|\|f\|_2}{\|\mathcal{C}_{out}f\|_2}\right\rfloor + 1,
\tag{177}
$$

we arrive at

$$
\|\mathcal{C}_{out}f\|_{L^\infty(I)} \leq c\,\|\mathcal{C}_{out}f\|_2\,\log\left(\frac{\|\mathcal{C}_{out}\|\|f\|_2}{\|\mathcal{C}_{out}f\|_2} + 1\right),
\tag{178}
$$

where $c > 0$ is a constant. Since every point in D^{out} is contained in some segment $I \subset D^{out}$ of length $a = \frac{1}{e}$, the lemma follows. $\qquad\square$

Now we proceed to the principal result of this section.

Theorem B.5 *Let ψ_n^{in}, ψ_n^{out} be the left singular functions of the operators $\mathcal{C}_{in}$ and $\mathcal{C}_{out}$, respectively. Then there exist constants $0 < q < 1$ and $c > 0$ such that*

$$
\|\psi_n^{in}\|_\infty \leq cn,
\tag{179}
$$

$$
\|\psi_n^{out}\|_\infty \leq cn,
\tag{180}
$$

for all $n = 1, 2, \ldots.$

44

Proof. Since $\mathcal{C}_{out}\phi_n^{out} = s_n\psi_n^{out}$, Lemma A.10 implies that, there is a constant $c_1 > 0$, such that

$$
\begin{aligned}
s_n\|\psi_n^{out}\|_\infty &\leq c_1 \, s_n\|\psi_n^{out}\|_2 \left(\log \frac{\|\mathcal{C}_{out}\|\|\phi_n^{out}\|_2}{s_n\|\psi^{out}\|_2} + 1\right) \\
&= c_1 \, s_n \left(\log \frac{1}{s_n} + \log\|\mathcal{C}_{out}\| + 1\right).
\end{aligned}
\tag{181}
$$

Now, due to Theorem A.6, there exists a constant $c > 0$, such that

$$
\|\psi_n^{out}\|_\infty \leq c\,n,
\tag{182}
$$

for n=1,2,.... It is easy to see, that Lemma A.10 holds with $\mathcal{C}_{out}$ replaced by $\mathcal{C}_{in} = \mathcal{C}_{out}^T$, and therefore this proof extends to the case of the left singular functions ψ_n^{in}. $\quad\square$

References

[1] M.ABRAMOWITZ, I.STEGUN, *Handbook of Mathematical Functions*, Applied Mathematics Series, National Bureau of Standards, Washington, DC, 1964.

[2] J.CARRIER, L.GREENGARD, V.ROKHLIN, *A Fast Adaptive Multipole Algorithm for Particle Simulations*. Technical Report 496, Yale Computer Science Department, 1985.

[3] I.GOHBERG, S.GOLDBERG, M.A.KAASHOEK, *Classes of Linear Operators, Vol.1.* Birkhäuser, 1990.

[4] L.GREENGARD, V.ROKHLIN, *A fast algorithm for particle simulations*. J. Comp. Phys., 73 (1987), pp. 325-348.

[5] P.R.HALMOS, V.S.SUNDER, *Bounded Integral Operators on L^2 Spaces*, Springer-Verlag, 1978.

[6] A.MARKUSHEVICH, *Theory of functions of a complex variable*. Chelsea Publishing Company, 1977.

[7] M.REED, B.SIMON, *Methods of modern mathematical physics, Vol.1.* Academic Press, 1980.

[8] V.ROKHLIN, *Rapid Solution of Integral Equations of Classical Potential Theory*. J. Comp. Phys., 60 (1985), p. 187-207.

[9] N.YARVIN, *Generalized Gaussian Quadratures and Fast Summation Schemes*. Ph. D. Dissertation, Yale University, in preparation.